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ANALYSIS AND ENVIRONMENTAL FATE OF AIR FORCE DISTILLATE AND HIGH DENSITY FUELS

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Five high density fuels (RJ-4, RJ-5, RJ-6, JP-9, and JP-10) and three distillate fuels were analyzed by capillary column gas chromatography (GC). The major components of the distillate fuels were identified by gas chromatography-mass spectrometry (GC-MS). The molecular weight of the isomers of the high density fuel components were also determined, but the structures of only a few components were assigned by comparing the GC retention times with authentic samples. —> cont

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The concentration and identity of the major water-soluble fuel components were also identified. The major aromatic components of the distillate fuels were benzene, toluene, ethylbenzene, the xylenes, 1,2,4-trimethylbenzene, naphthalene, and the methylnaphthalenes. The solubility of the high density fuel components was less than 0.02 mg liter^{-1} except for exo-tetrahydrodi(cyclopentadiene), which was less than 0.1 mg liter^{-1}. A correlation between the water solubility of the fuel component(s) and the fuel-water partition coefficient, K_{fw}, was found, where $K_{fw} = -0.799$ log S + 1.664 for JP-4, JP-5, and JP-8 at 20°C in deionized water at a fuel:water ratio of 1:1000.

The volatilization rates of the water-soluble components of JP-4, JP-8, and JP-9 were measured by preparing solutions of the fuel components in water, stirring at three stirring rates, and measuring the rate of decrease of the concentration of each component by GC as a function of time. The ratio of the component volatilization rate constant to the oxygen reaeration rate constant was measured. The average value of this ratio for the alkanes and substituted benzene components was 0.52 ± 0.09, which means that liquid phase mass transport resistance determines the volatilization rate. The estimated half-lives in the environment were 7 days in ponds, 1.5 days in rivers, and 6 days in lakes. The volatilization rates of naphthalenes, the methylnaphthalenes, and perhaps the tetra-substituted benzene derivatives were somewhat slower, suggesting that both gas and liquid phase mass transport resistance determine their volatilization rates.

The water-soluble components of JP-4 were photolyzed for 21 days in sunlight in deionized water, natural seawater, and water from a local pond. The alkanes, benzene, and the mono-substituted benzenes were stable. The di-, tri- and higher substituted benzenes photolyzed very slowly. The naphthalenes were transformed at rates that were competitive with their volatilization rates.

The distribution of the fuel components was estimated, using the method recently proposed by Mackay and Patterson. The alkanes should partition almost entirely into the atmosphere, the monoaromatics should be in both the air and water, and the naphthalene should partition into the water and the sediment phases. Adsorption of the alkanes and monoaromatics should not be a major environmental fate. Although quantitative rate estimates were not made, the primary environmental fate of many of the alkane and monoaromatic fuel components should be transport into the atmosphere where photolysis should be rapid.

It is recommended that the rate of dissolution in water and evaporation of the pure fuels be studied in detail because they may be the rate-limiting transport processes.

SUMMARY

Five high density fuels and three distillate fuels were analyzed by capillary column gas chromatography (GC). Many of the major components of the distillate fuels were identified by gas chromatography-mass spectrometry (GC-MS). The molecular weight of the isomers of the high density fuel components was also determined, but the structures of only a few components were assigned by comparing the GC retention times with authentic samples.

The concentration and identity of the major water-soluble fuel components were also identified. The major aromatic components were benzene, toluene, ethylbenzene, the xylenes, 1,2,4-trimethylbenzene, naphthalen, and the methylnaphthalenes.

The solubility of the high density fuel components was less than 0.02 mg liter^{-1} except for exo-tetrahydrodi(cyclopentadiene), which was less than 0.1 mg liter^{-1}. A correlation between the water solubility of the fuel component, S, and the fuel-water partition coefficient, K_{fw}, was found, where $K_{fw} = -0.799 \log S + 1.664$ for JP-4, JP-5, and JP-8 at 20°C in deionized water at a fuel:water ratio of 1:1000.

The volatilization rates of the water-soluble components of JP-4, JP-8, and JP-9 were measured by preparing solutions of the fuel components in water, stirring at three stirring rates, and measuring the rate of decrease of the concentration of each component by GC as a function of time. The ratio of the component volatilization rate constant to the oxygen reaeration rate constant, k_v^C/k_v^O, was measured. The average value of k_v^C/k_v^O for the alkanes and substituted benzene components was 0.52 ± 0.09, which means that liquid phase mass transport resistance determines the volatilization rate. The estimated half-lives in the environment were 7 days in ponds, 1.5 days in rivers, and 6 days in lakes. The volatilization rates of naphthalenes, the methylnaphthalenes, and perhaps the

tetra-substituted benzene derivatives were somewhat slower, suggesting that both gas and liquid phase mass transport resistance determine their volatilization rates.

The water-soluble components of JP-4 were photolyzed for 21 days in sunlight in deionized water, natural seawater, and water from a local pond. The alkanes, benzene, toluene, and the other mono-substituted benzenes were stable. The xylenes photolyzed slowly. The tri-substituted and higher benzenes and the naphthalenes were transformed at rates that were competitive with their volatilization rates.

The distribution of the fuel components was estimated, using the method recently proposed by Mackay and Patterson (1981). The alkanes should partition almost entirely into the atmosphere, the monoaromatics should be in both the air and water, and the naphthalenes should partition into the water and sediment phases. Adsorption of the alkanes and mono-aromatics should not be a major environmental fate. The primary environmental fate of many of the alkane and monoaromatic fuel components should be transport into the atmosphere where photolysis should be rapid.

It is recommended that the rate of dissolution and evaporation of the pure fuels be studied in detail because these processes may be the rate-limiting transport processes.

PREFACE

This research was conducted by SRI International, 333 Ravenswood Avenue, Menlo Park, California 94025, under contract No. F08635-80-C-0122, for the Headquarters Air Force Engineering and Services Center, Engineering and Services Laboratory, Environics Division, Environmental Chemistry Branch, Tyndall AFB, Florida 32403. Thomas B. Stauffer was the Project Officer.

The work was begun in August 1980 and completed in October 1981.

The authors acknowledge P. Boland and W. Peifer for their laboratory work early in the program, D. Thomas and C. Beeman for obtaining and interpreting the GC-MS data, and D. L. Haynes for his technical assistance throughout the program.

This report has been reviewed by the Public affairs Office and is releasable to the National Technical Information Service (NTIS). At NTIS it will be available to the general public, including foreign nations.

This report has been reviewed and is approved for publication.

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SECTION I

INTRODUCTION

In recent years considerable interest has been focused on the fate
of substances accidentally released to the environment. The broad
objective of this research project was to determine the aqueous environ-
mental chemistry of the Air Force hydrocarbon aviation fuels and to
provide information that can be used in environmental assessments. The
specific objectives were to:

- Develop simple procedures for analyzing five high density fuels
  and the major components (greater than 0.5% by weight) in
  three distillate fuels.

- Measure the "water-soluble" fuel components in deionized water
  and seawater.

- Measure the volatilization rates of the major fuel components in
  deionized water and seawater.

- Study the photolysis of the "water-soluble" fuel components in
  deionized water, a natural fresh water, and natural seawater.

The study did not include measurements of adsorption or biotransformation
of the water-soluble components.

As the project progressed, the problem of defining the water-soluble
fuel components arose because the fuels are all complex mixtures and the
solubility can be defined several ways. It was arbitrarily decided to
equilibrate the fuels at a fuel:water ratio of 1:1000. However, the
project scope was later modified, and the concentrations of the major
distillate fuel components, down to the detection limit of about 0.02 ppm,
were measured at 20°C and at fuel:water ratios of 1:10, 1:100, 1:1000,
and 1:10,000 in deionized water and artificial seawater.

The following fuels were studied (they were used as received from
the Air Force):

- High density fuels

  - JP-10: pure exo-tetrahydrodi(cyclopentadiene)

  - RJ-4: tetrahydrodi(methylcyclopentadiene)

  - RJ-5: pure endo, endo-dihydrodi(norbornadiene)

  - JP-9: 10% to 12% methylcyclohexane, 65% to 70% JP-10, and 20% to 25% RJ-5

  - RJ-6: blend of RJ-5 and JP-10

- Distillate fuels

  - JP-4: a mixture of gasoline and kerosene distillates

  - JP-5: a kerosene-based distillate that meets Navy flash point specifications

  - JP-8: a kerosene-based distillate that is similar to JP-5 and commercial Jet A-1.

SECTION II

BACKGROUND

1. FUEL STRUCTURES AND PROPERTIES

Two types of Air Force aviation fuels were studied in this research program: distillate fuels and high density ram jet fuels. The distillate fuels, JP-4, JP-5, and JP-8, are petroleum hydrocarbon fractions and contain alkanes from C_3 to C_{16}, cyclic alkanes, and substituted one- and two-ring aromatics. The detailed physical properties of these fuels are summarized in Appendix A.

The high density fuels studied, RJ-4, RJ-5, RJ-6, JP-9 and JP-10, are synthetic fuels. RJ-5 is formed by a Diels-Alder reaction of norbornadiene (I) followed by hydrogenation (Burdette et al., 1978). Some of the major possible isomers are shown below.
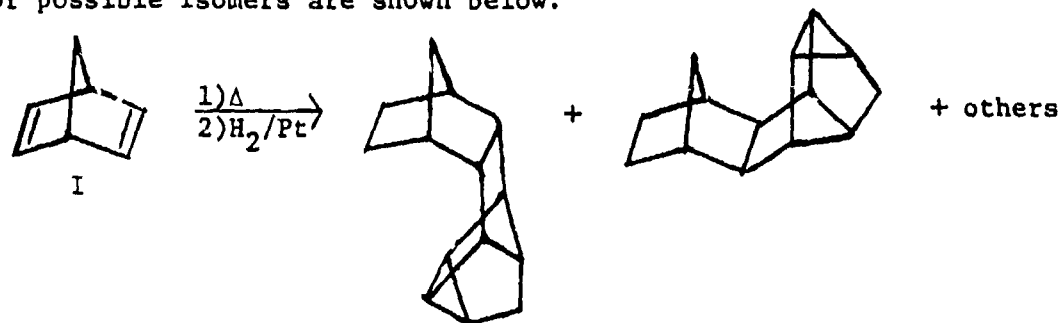
JP-10 formed by a Diels-Alder reaction of cyclopentadiene (II), followed by hydrogenation. The major isomers are:
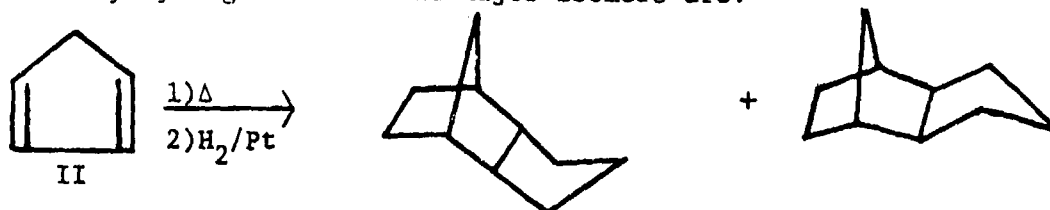
RJ-6 is a blend of RJ-5 (50%-55%) and JP-10 (40%-45%). JP-9 is a blend of RJ-5 (20%-25%), JP-10 (65%-70%), and methycyclohexane (10%-12%).

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RJ-4 is formed by a Diels-Alder reaction of methylcyclopentadiene (III) followed by hydrogenation. The backbone of the dimers are similar to the isomers of JP-10, but the addition of the methyl groups increases the possible number of isomers by a factor of four or more.
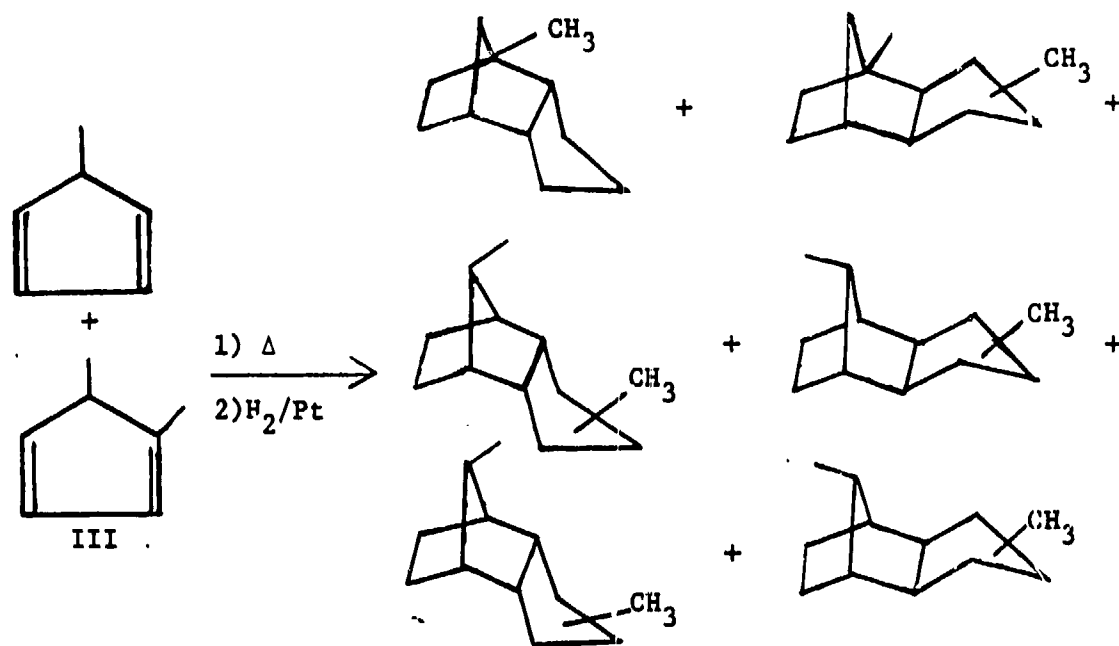
The high density fuels also contain an antioxidant: RJ-4 contains 2,6-di-t-butyl-4-methyl phenol (IV), and RJ-5 and RJ-6 may contain IV, 2,4-dimethyl-6-t-butylphenol (V), or 2,6-di-t-butylphenol (VI).
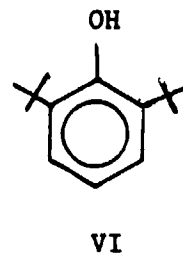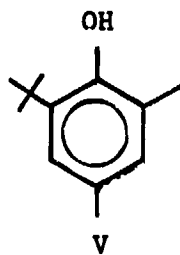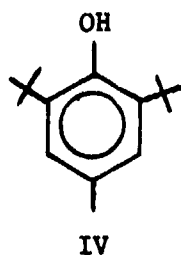
The density of the fuels is an important physical property when the partitioning of fuel components between the bulk fuels and water is studied. The densities of the fuels, as summarized in Table 1, are taken from the physical property data provided by the Air Force and included in Appendix A.

TABLE 1. DENSITIES OF FUELS STUDIED

Fuel	Gravity	Specific Gravity at 60°F
JP-4	54.3	0.7616
JP-5	42.6	0.8128
JP-8	42.3	0.8142
RJ-4	21.8	0.9230
RJ-5	NA	1.0890
RJ-6	8.2	1.0129
JP-9	17.8	0.9368*
JP-10	19.2	0.9390

*Estimated from the densities of
methylcyclohexane, JP-10, and RJ-5.

2. ANALYSIS OF DISTILLATE FUELS

Analysis of petroleum-derived distillate fuels has been the subject
of intense research for years. In this study, the objective was to identify
the major hydrocarbon components greater than 0.5% by weight. Therefore,
our literature review focused on chromatographic separation techniques
such as liquid-liquid-solid chromatography to obtain major fuel fractions,
followed by high resoltuion GC and GC-MS to separate and identify the
individual fuel components.

Suatoni and coworkers (1975a, 1975b) have described two high perfor-
mance liquid chromatography (HPLC) methods for separating fuel fractions
into alkanes (saturated), olefins, and aromatics. They proposed that
this method could be used as a substitute for the ASTM D1319 standard
method (ASTM, 1973). However, the amount of fuel used in this method is
small, so the sample available for subsequent GC analysis is also small.
Also, the sample is in methanol-water or a fluorocarbon after elution from
the HPLC column, and extraction into a solvent suitable for the GC analysis
would be difficult. A similar method was proposed by Stevenson (1971).

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Alternative liquid-solid chromatographic separation methods have been reported by Hirsch et al (1972) (and numerous studies cited in this reference). Hirsch's method involves the use of a dual-packed column (2.54-cm OD by 244-cm high) containing silica gel and alumina. The hydrocarbons are eluted with n-pentane to elute the saturated alkanes, 5% benzene in n-pentane to elute the monoaromatics, 15% benzene in n-pentane to elute the diaromatics, and 20% ether-20% benzene-60% methanol to elute the polycyclic aromatics. Although the method gives excellent separations, it is very cumbersome and time consuming.

A much simpler method has been suggested by Warner (1976), who separated aliphatics, monoarmatics, and polycyclic aromatics by liquid-solid chromatography on silica gel. The 0.9 x 25 cm column was packed wet in petroleum ether. The saturated hydrocarbons were eluted with 25 ml petroleum ether. Fraction 2 contained the mono- and diaromatics and most of the olefins. Fraction 3 contained the triarmoatics. The method appears to be very simple and gives an excellent separation of the saturated hydrocarbons from the aromatics.

Solash and Taylor (1976) used silica gel chromatography to separate aliphatics from aromatics in shale oil derived JP-5. Gearing et al (1980) used a similar method to separate the hydrocarbons in No. 2 fuel oil However, the experimental details were not reported in either case.

High resolution GC analysis of the more volatile petroleum distillates are commonplace methods within the petroleum industry. The classic reference is by Sanders and Maynard (1968), who used squalane coated on a stainless steel capillary column. More recently, Whitmore (1979) published an extensive list of hydrocarbons in their order of elution from metal squalane columns. This technique has a major disadvantage, however, in that squalane columns cannot be heated to more than 120°-140°C, and the use of solvents such as hexane, methylene chloride, or carbon disulfide is not practical.

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About two-thirds of the way through this project, data were received from Major Donald Potter, U.S. Air Force, Wright-Patterson AFB. Major Potter and his staff chromatographed authentic samples of about 75 hydrocarbons on fused silica capilliary columns coated with OV-101 and OV-17 and calculated the Kovats indices (see Kovats, 1958, and Section IV) for the compounds. Then they analyzed fuel samples from the same batches of JP-4, JP-5, and JP-8 as studied in this work. These data were made available to use after we had identified the major fuel components by capilliary column GC and GC-MS, as described in Section IV 2.

3. ANALYSIS OF WATER-SOLUBLE FUEL COMPONENTS

a. Theory

The water-soluble fraction of a hydrocarbon fuel is in fact the equilibrium partitioning of the individual fuel components between the hydrocarbon-saturated aqueous phase and the water-saturated hydrocarbon phase. The physical chemistry principles are the same as for the octanol-water partitioning of pure chemicals, except that the organic phase is a complex mixture. As discussed in detail by Mackay and Patterson (1977, 1981), the hydrocarbon fuel-water mixture will be at equilibrium if the fugacities of each of the ith components (f_i) are equal in the hydrocarbon and aqueous phases. Thus

$$f_i^O = f_i^W \tag{1}$$

Fugacity can be considered an escaping tendency of the substance from a phase and has units of pressure. It is an especially useful concept because at low concentrations (ideal solutions) fugacity is proportional to concentration. The proportionality constant between the fugacity and concentration is called the fugacity capacity, where

$$f = z \, C \tag{2}$$

In an ideal solution, the fugacity of a solute is

$$f = x \, \gamma \, f^R \tag{3}$$

where x is the mole fraction, γ is the activity coefficient, and f^R is the

reference fugacity. If the Raoult's law convention is used to define γ,

$$\gamma \to 1 \text{ as } x \to 1 \tag{4}$$

Then f^R is the vapor pressure of the pure liquid component, P^S, and

$$f = x \, \gamma \, P^S \tag{5}$$

If an organic solute is partitioned between an organic solvent and water, and the system is at equilibrium

$$f_i^O = f_i^W \tag{6}$$

$$x_i^O \gamma_i^O \, P_i^S = x_i^W \, \gamma_i^W \, P_i^S \tag{7}$$

$$x_i^O \, \gamma_i^O = x_i^W \, \gamma_i^W \tag{8}$$

Also, the equilibrium can be expressed in terms of a partition coefficient, K_{ow}, where

$$K_{ow} = C^O/C^W \tag{9}$$

From equations (2) and (9), at equilibrium

$$f_i^O = f_i^W = C_i^O/z_i^O = C_i^W/z_i^W \tag{10}$$

$$K_{ow} = C_i^O/C_i^W = z_i^O/z_i^W \tag{11}$$

The fugacity coefficients, z_i^O and z_i^W, are equal to $1/H$ in both phases, because

$$z = C/f = C/P^S = 1/H = x/v \, f = 1/v \, \gamma \, P^S \tag{12}$$

$$\tag{13}$$

where v is the molar volume of the solute. Then,

$$K_{ow} = v_i^W \, \gamma_i^W / v_i^O \, \gamma_i^O \tag{14}$$

because the vapor pressure, P^S cancels. This development has been used by Mackay and Patterson to discuss the partitioning of a solute between octanol and water (Mackay, 1977; Mackay and Patterson, 1981), but it should

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apply just as well to the partitioning of a fuel component between the bulk fuel (the organic phase) and water. Mackay also points out that v_i^w and v_i^o are constants and that γ_i^o is fairly constant in octanol (about 1-10). Since a dilute solution of one hydrocarbon in another is nearly an ideal solution, γ_i^o should be about 1 if the organic phase is a hydrocarbon fuel. This means that the partitioning of a fuel component between a bulk fuel and water is governed almost entirely by γ_i^w.

Mackay et al (1980) and Banerjee et al (1980) have developed correlations of K_{ow} for octanol and the aqueous solubility of an organic solute. Mackay's equation is:

$$\ln K_{ow} = 7.494 - \ln C^s \text{ (for liquids)} \tag{15}$$

$$\ln K_{ow} = 7.494 - \ln C^s + 6.79 (1 - T_M/T) \text{ for solids} \tag{16}$$

Banerjee's equation is:

$$\log K_{ow} = 6.5 - 0.89 \log C^s - 0.015 T_M \tag{17}$$

where T_M is the melting point, which is in Kelvin in Mackay's equation and in Celsius in Banerjee's. If the substance is a liquid at 25°C, T_M = 0 in Mackay's equation and 25°C in Banergee's. It should be possible to develop similar equations for the partitioning of a hydrocarbon solute between the bulk fuel and water.

Mackay and Patterson (1981) have derived the value of z for a chemical in the different compartments of the biosphere:

- Water: $z_w = 1/H$ (18)
- Air: $z_a = 1/RT$ (19)
- Sorbed phases (sediments): $z^s C_s/HC_w = K_p \rho_s/H$ (20)
- Biota: $z_b = K_b \rho_b/H$ (21)

where K_p is the adsorption partition coefficient on the suspended sediments, ρ is the density of the sediment, or biota and K_b is the adsorption partition coefficient on the biota (in water). (See Mackay and Patterson, 1981, for an excellent discussion of these concepts.) They have also used this basic approach to develop several simple models of the environmental fate of a chemical. The basic assumptions of this

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model are that the environment can be divided into separate compartments and that the rates of loss or transformation of the chemical in each compartment are independent. In the level I model, they calculate the partitioning of a chemical among the air, soil, water, biota, suspended sediments, and sediments. In the level II approach, the loss rate from each compartment is also calculated. A simple application of these models is illustrated in Section V.1 of this report.

b. Laboratory Measurements

During the literature review, several methods for determining water-soluble hydrocarbons were found. Three basic analytical methods are generally used: direct aqueous injection and analysis by GC or HPLC, extraction followed by GC analysis, and purge-trap.

Dell'aqua et al (1976) described an extraction method for analyzing the water-soluble portion of gasolines. A 2-liter water sample was acidified and extracted with 10 ml solvent. The extract was dried over sodium sulfate and analyzed on 2-m packed GC columns using a flame ionization detector (FID). The authors commented that, although CS_2 could be used, hexadecane was the best solvent because it did not interfere with the FID response to the lower molecular weight fuel components.
* This method was used as a qualitative method for fingerprinting groundwater samples that had been contaminated with gasoline. Identification of the major fuel components was not adequate for the work described in this report because the GC column resolution was poor. However, the use of hexadecane as an extracting solvent was an excellent idea.

Price (1976) reported an extensive study of the solubility of pure hydrocarbons and petroleum fractions in water. He used 0.32-cm (1/8-in.) copper GC columns packed with uncoated Poracil C® or Poracil F® for the analysis. The hydrocarbon-to-fuel ratio and sample GC traces of the petroleum fractions were not reported. However, the resolution of the column would be poor. The solubility data for the pure hydrocarbons at 25°C were determined by equilibrating the hydrocarbon with the fuel in screw-cap test tubes fitted with Teflon® or aluminum foil lined septa. The samples were equilibrated, apparently without stirring, for four days.

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Then the aqueous phase was sampled with a syringe needle, which pierced the septa and the remaining hydrocarbon phase. The aqueous sample was anlayzed directly by GC. Price reported that equilibrium was reached in two to four days. The solubility data for the petroleum fractions are not usable because the hydrocarbon-to-water ratio and the solubility of individual components were not reported.

McAuliffe reported the solubility in water of 65 hydrocarbons (McAuliffe, 1966) and n-alkanes (McAuliffe, 1969). Excess hydrocarbon was equilibrated with water by shaking for 1 hour or stirring for 1 day. The samples were allowed to stand for two days before analysis by GC. No hydrocarbon droplets were visible by phase contrast microscopy, which means that the droplets, if present, were less than 0.2 μm. The data from Price (1976) and McAuliffe (1966, 1969) are in excellent agreement and are summarized in Table 2.

Berry and Stein (1977) described a direct aqueous injection method for determining the water-soluble fraction of gasoline. The hydrocarbon and fuel samples were equilibrated in 1 liter of water with rapid stirring The solution was then poured into a 1-liter separatory funnel and allowed to separate for 16 to 18 hours. About 950 ml of the aqueous fraction was removed from the separatory funnel and "...mixed for 2 hours to disperse the water soluble components." It is our opinion that this last comment puts the entire study of Berry and Stein in question, because the implication of dispersing the water-soluble fraction is that the pure fuel or hydrocarbon was still present in the aqueous fraction and the rapid stirring of the aqueous phase means that the water-soluble components would be rapidly volatilized from the solution of be equilibrated with the headspace if the vessel were closed. The samples were analyzed by direct aqueous injection on packed GC columns using a FID.

Klein and Jenkins (1981) described the purge and trap method (Bellar and Lichtenberg, 1974) and a pentane extraction method for determining the water-soluble fraction of distillate jet fuels. The water-soluble fraction was produced by a continuous flow solubilizer described by Krugel et al. (1978). The apparatus consists of a series of vertical

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TABLE 2. SOLUBILITIES OF PURE HYDROCARBONS IN WATER AT 25°C

Aliphatic Hydrocarbons	Solubility (mg liter^{-1})	
	a	b
n-Pentane	39.5	38.5
n-Hexane	9.47	9.52
n-Heptane	2.24	2.93
n-Octane	0.431	0.66
n-Nonane	0.122	0.220
2,3-Dimethylbutane	19.1	--
2,2-Dimethylbutane	21.2	18.4
2-Methylpentane	13.0	13.8
3-Methylpentane	13.1	12.8
2,4-Dimethylpentane	4.41	4.06
2,2-Dimethylpentane	4.40	--
2,3-Dimethylpentane	5.25	--
3,3-Dimethylpentane	5.94	--
2,2,4-Trimethylpentane	1.14	2.2
2,3,4-Trimethylpentane	1.36	--
Isopentane	48.0	47.8
2-Methylhexane	2.54	--
3-Methylhexane	2.64	--
3-Methylheptane	0.792	--
4-Methyloctane	0.115	--
Indane	88.9	--
Cyclopentane	160.0	156.0
Methylcyclopentane	41.8	42.0
1,1,3-Trimethylcyclopentane	3.73	--
Cyclohexane	66.5	55.0
Methylcyclohexane	16.0	14.0
1,4-trans-Dimethylcyclohexane	3.84	--
1,1,3-Trimethylcyclohexane	1.77	--

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[a] Price (1976).

[b] McAuliffe (1966, 1969).

TABLE 2. SOLUBILITIES OF PURE HYDROCARBONS IN WATER A1 25°C (Concluded)

Aromatics	Solubility (mg liter^{-1})	
	a	b
Benzene	1740	1780
Toluene	554	515
m-Xylene	134	--
c-Xylene	167	175
p-Xylene	157	--
1,2,4-Trimethylbenzene	51.9	57
1,2,4,5-Tetramethylbenzene	3.48	--
Ethylbenzene	131	152
i-Propylbenzene	48.3	50
i-Butylbenzene	10.1	--
Naphthalene	34.1[c]	

[c]Mackay and Shiu (1977).

columns containing the fuel. Water is dripped slowly through the fuel and passes successively from one column to the next. The authors reported that there were significant changes in the composition of the water-soluble fraction. It is not possible to estimate the fuel-to-water ratio in their apparatus. Additional details of the composition changes are reported by Klein and Jenkins (1981).

Klein and Jenkins (1981) also showed that the GC chromatograms of the pentane extracts and purge-trap analyses of JP-8 water-soluble fraction were very similar. However, with JP-4, the pentane obscured the low molecular weight (C_4-C_6) hydrocarbons of JP-4. Klein and Jenkins also concentrated the JP-4 and petroleum-derived JP-8 pentane extracts before analysis and lost 30% to 50% of hydrocarbons, compared with the recovery by purge-trap. Unfortunately, the authors did not identify or quantitate the fuel components.

Laughlin et al (1979) determined the water-soluble fraction of No. 2 fuel oil (American Petroleum Institute reference oil III) using hexane extraction and ultraviolet spectrocopy. They stated that the major components of the hexane extracts were naphthalene (λ_{max} = 221 nm), methylnaphthalenes (λ_{max} = 224 nm), and dimethylnaphthalenes (λ_{max} = 228 nm). GC analysis was not reported.

Gearing et al (1980) reported the extraction and capillary column GC analyses of the water-soluble fractions of No. 2 fuel oil. They used petroleum ether to extract the fuel, column chromatography on silica gel or silica gel/alumina to separate the aliphatic and aromatic fractions, and SE-52 and OV-101 coated glass capillary GC columns. The identification of specific peaks was not reported.

4. VOLATILIZATION FROM WATER

The volatilization rate of a chemical that is dissolved in water is a first-order process. Therefore, the volatilization rate is

$$R_v = \frac{dC}{dt} = -k_v \, C \qquad (22)$$

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where

$$k_v = \frac{1}{L}\left(\frac{1}{k_\ell} + \frac{1}{H\,k_g}\right)^{-1} \qquad (23)$$

where C is the concentration of the chemical in water (moles liter^{-1} = M) k_v is the volatilization rate constant (hr^{-1}), L is the solution depth (cm), k_ℓ is the liquid phase mass transport coefficient (cm hr^{-1}), H is Henry's constant (unitless as defined here), and k_g is the gas phase mass transport coefficient (cm hr^{-1}). The derivation of these equations, which are an expression of the two-film theory, has been described by Whitman (1923), Liss and Slater (1974), Mackay and Lieonen (1975), Smith and Bomberger (1980), Smith et al (1980, 1981). The major assumptions are as follows:

- The gas and liquid bulk phases are homogeneous (well-mixed).

- A stagnant boundary layer exists in both phases near the inter-face, where the turbulence is laminar and mass transport across the boundary layers is only by diffusion.

- At the air-water interface the chemical is at equilibrium in the gas and liquid phases as determined by Henry's law.

- Henry's constant is defined by

$$C_g = H\,C_\ell \qquad (24)$$

where C_g and C_ℓ are the concentrations of the chemical in the gas and liquid phases.

Typical values of the mass transfer coefficients for the open ocean were estimated by Liss and Slater (1974). They suggested that $k_\ell \approx 20$ cm hr^{-1} for CO_2 and $k_g \approx 1000$ to 3000 cm hr^{-1} for water. If H is greater than about 5×10^{-2}, the second term of equation (23) is smaller than the first term, and liquid phase mass transport resistance determines the volatilization rate. Similarly, if H is less than about 5×10^{-4}, the first term of equation (23) is smaller than the second and gas phase mass transport resistance controls the volatilization rate. If H is between 5×10^{-2} and 5×10^{-4}, both terms are important.

The value of H can be measured by several methods, such as parti-tioning the chemical between the air and water phases (McAuliffe, 1971) or by stripping an aqueous solution with air (Mackay et al., 1979).

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Typical values of H for hydrocarbons in the distillate jet fuels are summarized in Table 3. If measured values of H are not available, they can be estimated from the vapor pressure and solubility in water of the pure material (Mackay and Wolkolf, 1973).

The values of H for the representative hydrocarbons that are present in the distillate fuels are much greater than 5×10^{-2}, suggesting that the volatilization rates of the distillate fuels should be controlled by liquid phase mass transport resistance. Vapor pressure and solubility data for the high density fuels are not available, but the fuels are composed of C_{10}, C_{12}, or C_{14} hydrocarbons. A value of H for n-decane is available (499, Table 3), and the values of H for the high density fuels should be of similar magnitude. Thus, the volatilization rates of the high density fuels and all the components of the distillate fuels, except naphthalene and its derivatives, are expected to be controlled by liquid phase mass transport resistance.

If liquid phase mass transport resistance controls the volatilization rate, equation (23) reduces to

$$k_v = k_\ell/L \tag{25}$$

(Smith et al , 1950 and references therein) because the second term in equation (23) is much smaller than the first term. Furthermore, the mass transfer coefficients are equal to

$$k_\ell = D_\ell/\delta_\ell \tag{26}$$

$$k_g = D_g/\delta_g \tag{27}$$

where D is the diffusion coefficient of the chemical in water or air and δ is the boundary layer thickness in the water or gas phase. The ratio of the volatilization rate constants for two substances such as the fuel component and oxygen which are both controlled by liquid phase mass trans- transport resistance, will be a constant, since

$$k_v^C/k_v^O = k_\ell^C/k_\ell^O = D_\ell^C/D_\ell^O = \text{constant} \tag{28}$$

The superscripts C and O refer to the chemical or fuel component and oxygen, respectively.

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TABLE 3. HENRY'S CONSTANTS FOR SELECTED HYDROCARBONS

	Henry's Constant (unitless)
Aliphatic hydrocarbons	
n-Pentane	51.6^a
n-Hexane	49.0^b
n-Decane	499^a
Cyclopentane	3.76^a
Cyclohexane	$7.88^{a,b}$
Methylcyclohexane	15.4^a
Aromatic hydrocarbons	
Benzene	0.230^c
	0.219^a
Toluene	$0.272^{a,b}$
	0.275^c
Ethylbenzene	0.349^c
	0.339^b
Naphthalene	0.020^c

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[a] McAuliffe, 1980.
[b] McAuliffe, 1971.
[c] Mackay, et al., 1979.

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The validity of equation (28) has been demonstrated in our laboratory, as well as in several others (Smith et al , 1980 and references therein). For instance, the data summarized in Figure 1 show that for benzene the ratio k_v^C/k_v^O is independent of temperature, salinity, surfactant, and stirring rate (liquid phase turbulence), within experimental error (Smith et al , 1980).

Oxygen is a particularly convenient choice for the reference compound. It has a high volatility ($H \sim 6.6$, which was estimated from the solubility of oxygen in water, Weast, 1973), and its concentration in water is easily measured with a dissolved oxygen analyzer. Representative values of k_v^O in various environmental situations are available (Table 4). The value of k_v^O is determined by measuring the oxygen reaeration rate in a solution that has been purged with N_2 or He to remove the dissolved oxygen. Then

$$\frac{d[O_2]}{dt} = k_v^O \left([O_2]_{sat} - [O_2]_t\right) \tag{29}$$

where the subscripts sat and t refer to the dissolved oxygen concentration when the solution is saturated or at time t. Then, k_v^O is the slope of a plot of $\ln\left([O_2]_{sat} - [O_2]_t\right)$ versus t.

Since the ratio k_v^C/k_v^O is constant (if $H > 5 \times 10^{-2}$), then

$$\left(k_v^C/k_v^O\right)_{env} = \left(k_v^C/k_v^O\right)_{lab} \tag{30}$$

and

$$\left(k_v^C\right)_{env} = \left(k_v^C/k_v^O\right)_{lab} \left(k_v^O\right)_{env} \tag{31}$$

The value of $\left(k_v^C/k_v^O\right)_{lab}$ is measured by measuring the volatilization rate of the chemical and the oxygen reaeration rate at the same time. Values of $\left(k_v^O\right)_{env}$ have been estimated several ways, and typical values have been suggested by Smith et al (1980), as summarized in Table 4. Thus, this method is a very simple way to estimate the volatility of the water-soluble fraction of the fuels from water.

18
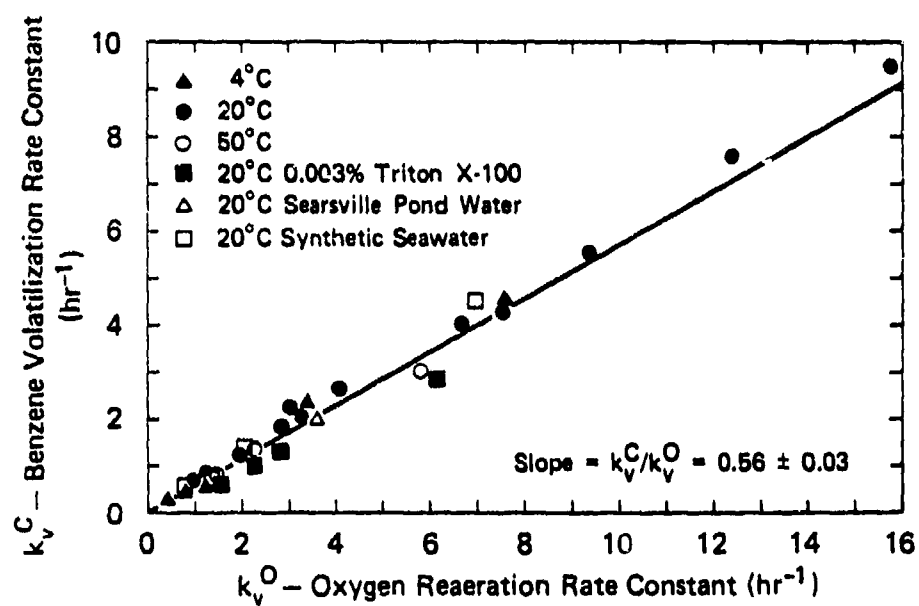
Figure 1. Volatilization Data for Benzene

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TABLE 4. OXYGEN REAERATION RATE CONSTANTS (k_v^O) IN REPRESENTATIVE WATER BODIES

	Literature Values (day^{-1})	Typical Values Selected by Smith et al. (1980)		
		k_v^O (day^{-1})	k_v^O (hr^{-1})	L (cm)
Pond	0.11-0.23[a]	0.19	0.0080	200
River	0.2[b], 0.1-9.3[c]	0.96	0.040	300
Lake	0.10-0.30	0.24	0.010	500

[a]Metcalf and Eddy (1972).
[b]Grennev et al. (1976).
[c]Langbein and Durum (1967).

SECTION III

METHODS AND RESULTS

1. GENERAL METHODS

The experimental methods and results are summarized in this section.
Details are given in the appendices. Appendix A gives the results of
standard method of analysis of the fuels supplied by the Air Force. A
combination of capilliary column GC, liquid solid column chromatography,
and GC-MS was used by SRI to identify the principal fuel components.
The details of the experimental methods and instrument conditions are
given in Appendix B; the GC and GC-MS traces and complete tables of the
experimental data are included in Appendix C.

Warner's (1976) method for separating the aliphatic monoaromatic
and polycyclic aromatic hydrocarbon fractions of distillate mixtures
was used in this study because of its simplicity. A batch of 90 to 200
mesh silica gel was washed with methylene chloride and activated at 155°C.
A 100-µl aliquot of the fuel was separated on 10 g of silica gel in a
0.9-cm-I.D. column. The aliphatic hydrocarbons were eluted with 25 ml
hexane; then the substituted benzenes and naphthalenes were eluted with
25 ml of 20% methylene chloride-80% hexane. A second 25-ml volume of
20% methylene chloride-80% hexane would contain the higher polycycylic
aromatics, but they were not observed. The concentrations of the fuel
components in the column eluates were high enough that they could be
analyzed by GC and GC-MS without concentration.

Both the fuels and the column eluates were analyzed by capillary
column GC and by capillary column GC-MS. Initial results were obtained
with a 25-m by 0.21-mm-ID SP-2100 column, but most of the results reported
here were obtained using a 30-m by 0.25-mm-ID SE-30 column. Both SP-2100
and SE-30 are methyl silicone liquid phases. The results of the GC-MS
analyses of the entire fuel and the fractions showed that separation of
the aliphatics and aromatic components was 100% within experimental error.

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GC analyses of the pure fuels were made by both split and splitless injection of the fuels diluted in either carbon disulfide (CS_2) or hexane. In the split injection mode, a 0.1-μl sample was injected. Most of the carrier gas in the injector was vented so that only 0.5% of the injected sample passed through the GC column. Thus, neat or concentrated samples could be analyzed.

In the splitless mode (Grob and Grob, 1974), the entire injected sample was passed onto the column, and the solvent effect on the liquid phase of the column caused the sample to concentrate at the head of the column. Therefore, it is the method of choice for the analysis of aqueous extractions. However, the disadvantage of the method is that the solvent peak obscures the light end components so that cyclohexane and benzene are the first quantifiable peaks.

The results of the split injection GC analyses of the distillate fuels are shown in Figures 2 through 4. The results of the splitless injection GC analyses of the high density fuels are shown in Figures 5 through 9.

2. IDENTIFICATION OF FUEL COMPONENTS

In the distillate fuels analyses, the Kovats retention indexes (Kovats, 1958) were calculated using the following equation:

$$I = 100 \frac{\log V_{N(substance)} - \log V_{N(n-Cz)}}{\log V_{N(n-Cz+1)} - \log V_{N(n-Cz)}} + 100z \qquad (32)$$

where V_N = net retention volume, n-Cz = n-paraffin with z carbon atoms, n-Cz+1 = n-paraffin with z + 1 carbon atoms and z = an integer where

$$V_{N(n-Cz)} \leq V_{N(substance)} \leq V_{N(n-Cz)+1} \qquad (33)$$

A solution of n-alkanes from n-heptane to n-octadecane was prepared in CS_2 and analyzed separately to obtain the retention times of each n-alkane. Then the solution was co-injected with a solution of each fuel, and the Kovats index of each peak was calculated. Once these data were tabulated, it was possible to identify the GC peaks in the extracts

22
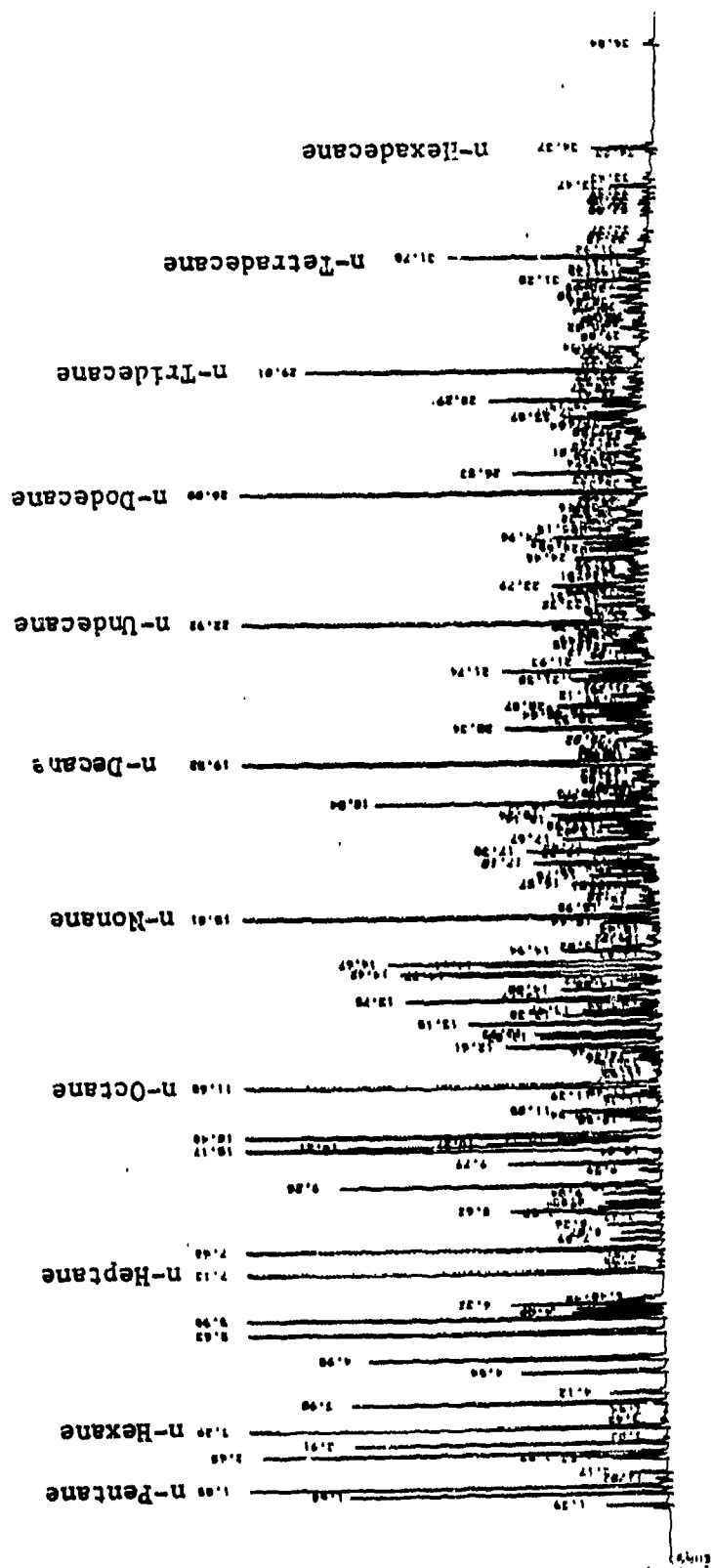
Figure 2. Split Injection GC Analysis of JP-4 (0.1 µl split 200:1)
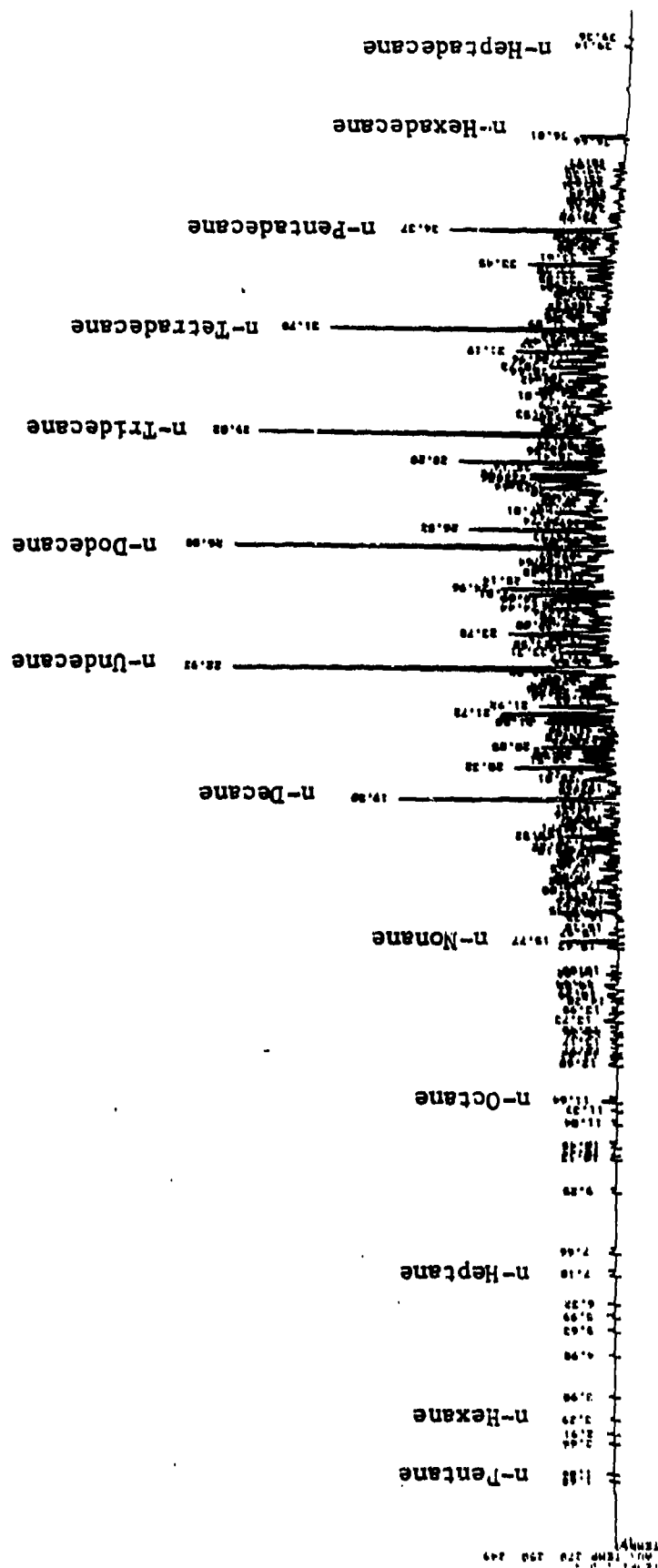
Figure 3. Split Injection GC Analysis of JP-5 (0.1 μl split 200:1)

24
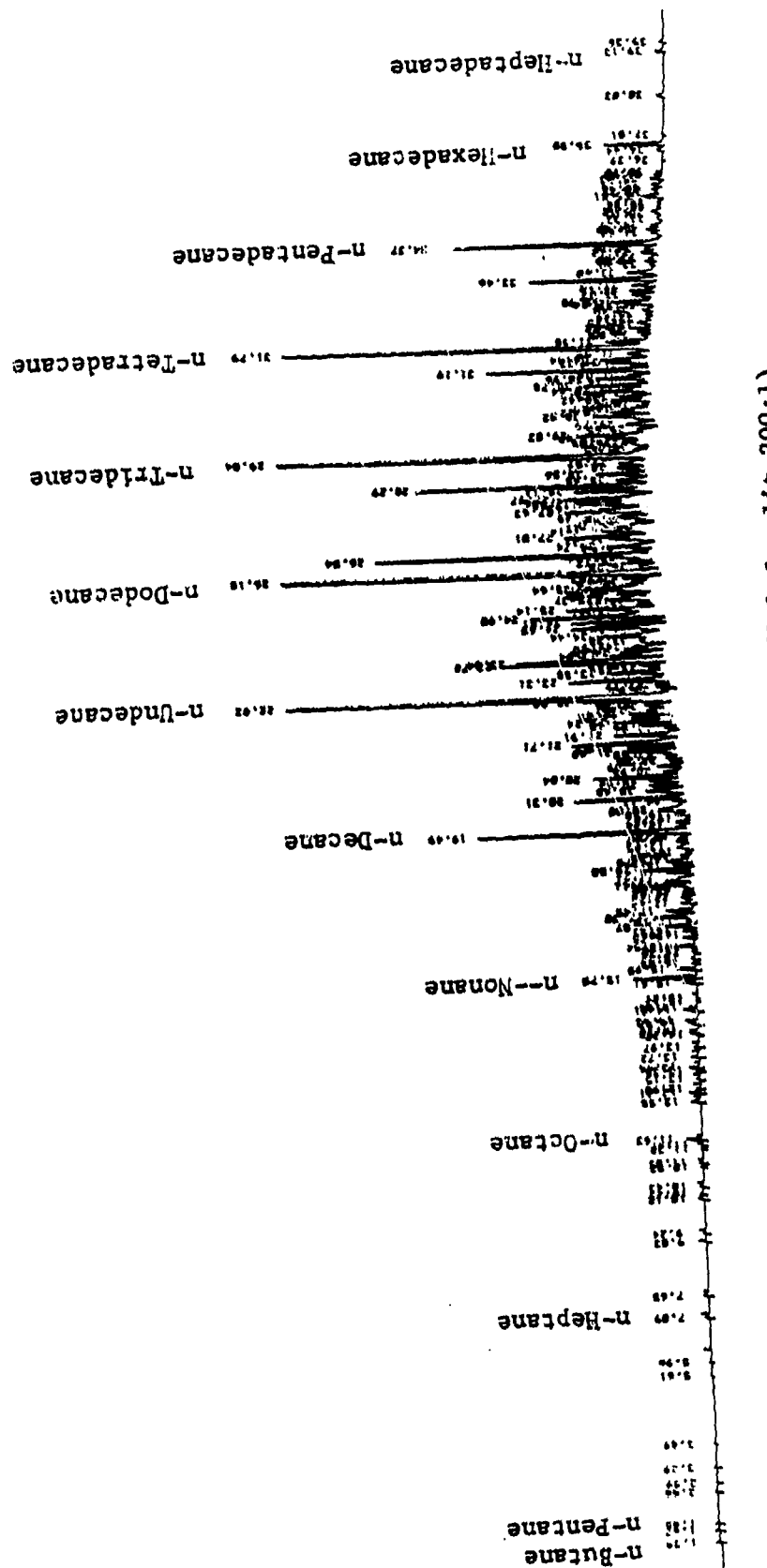
Figure 4. Split Injection GC Analysis of JP-8 (0.1μl split 200:1)
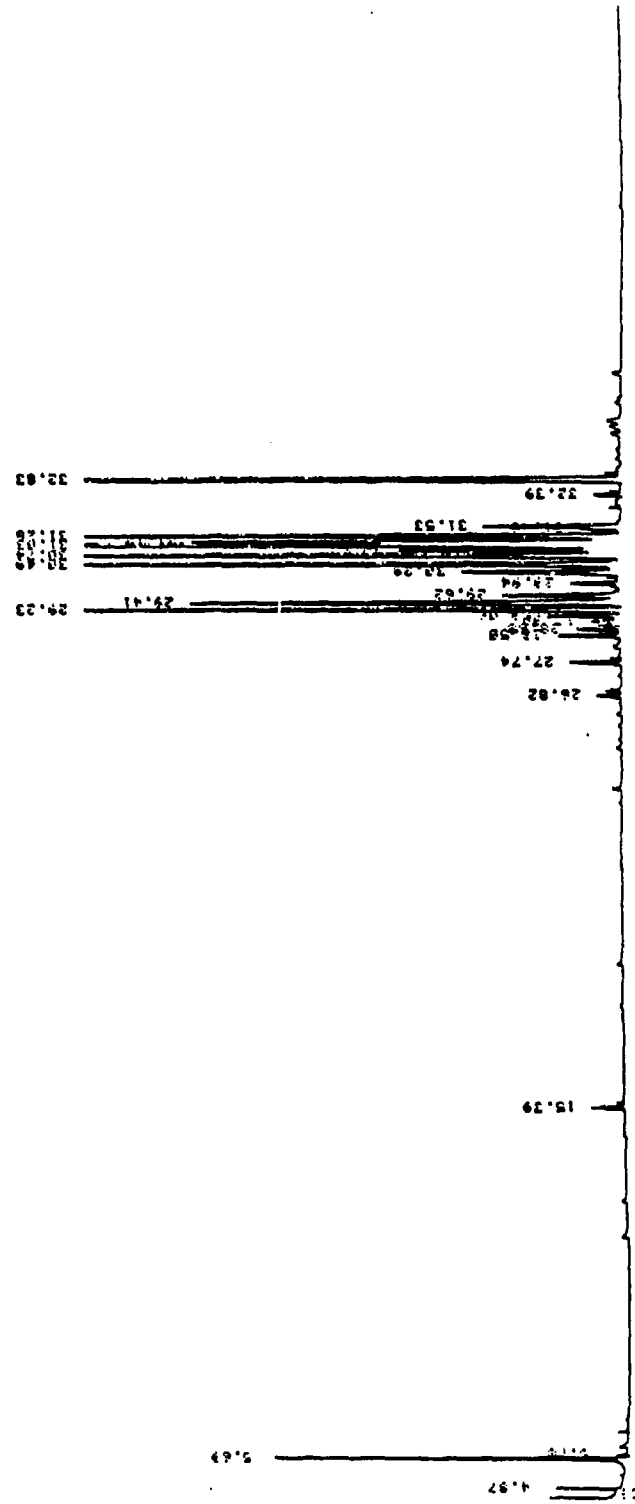
Figure 5. Splitless Injection GC Analysis of RJ-4
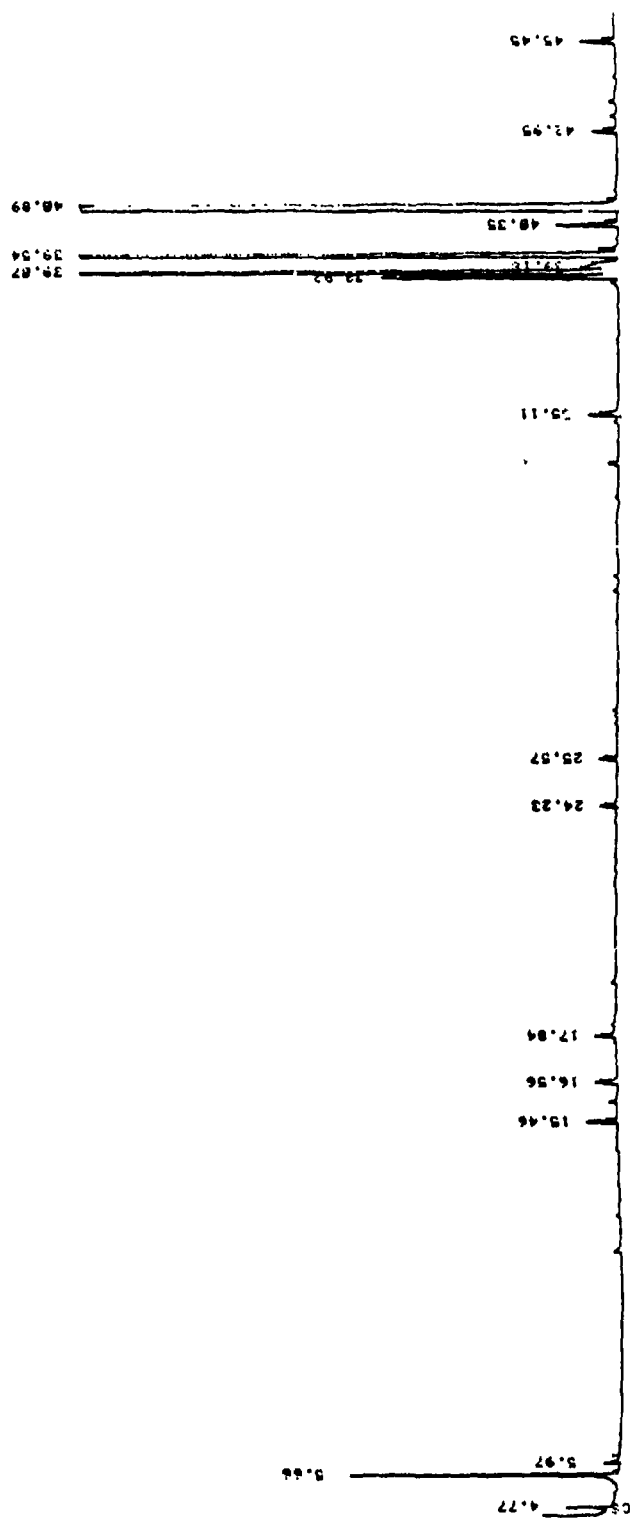
Figure 6. Splitless Injection GC Analysis of RJ-5
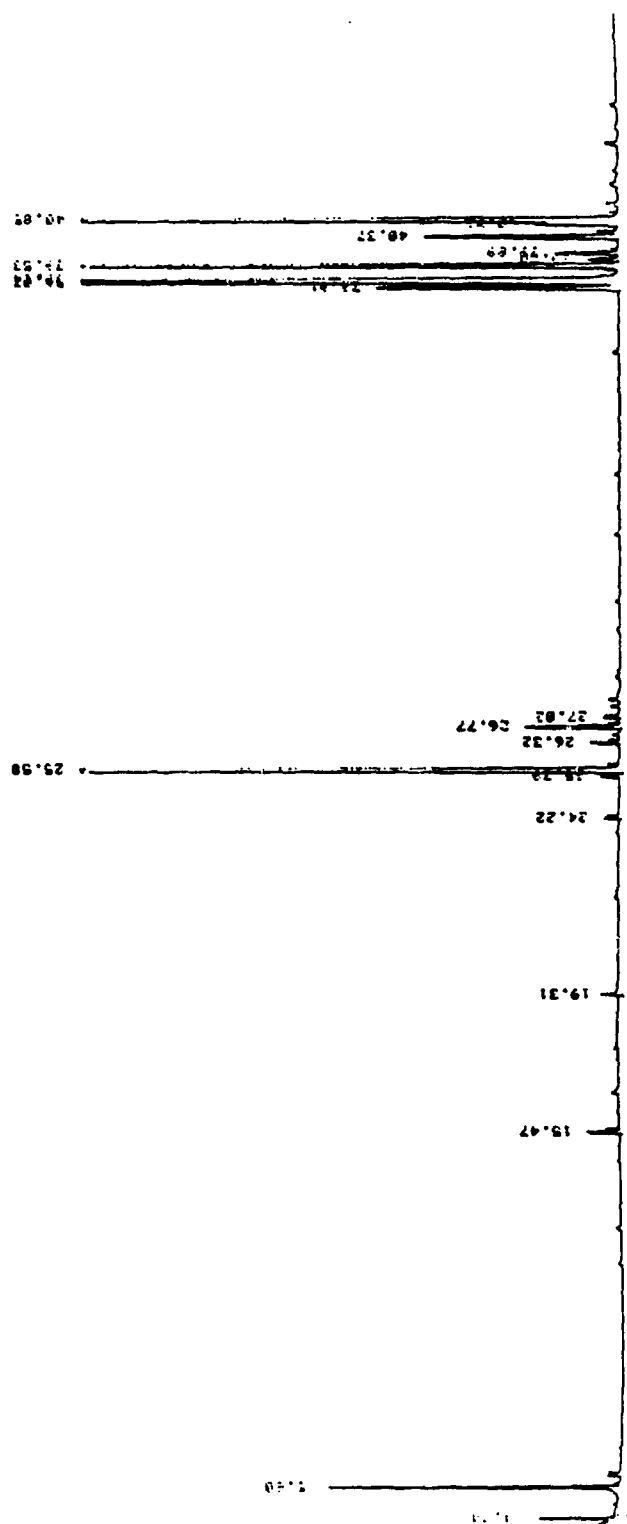
Figure 7. Splitless Injection GC Analysis of RJ-6

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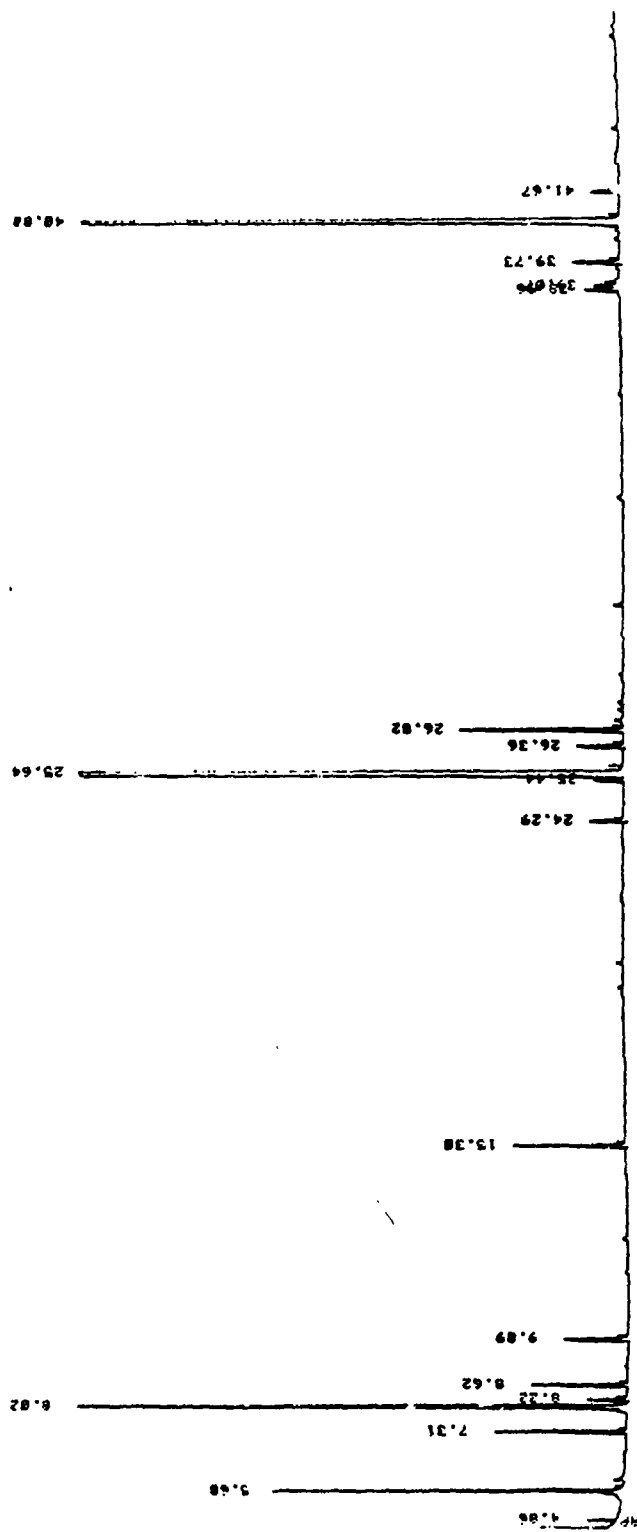
Figure 8. Splitless Injection GC Analysis of JP-9
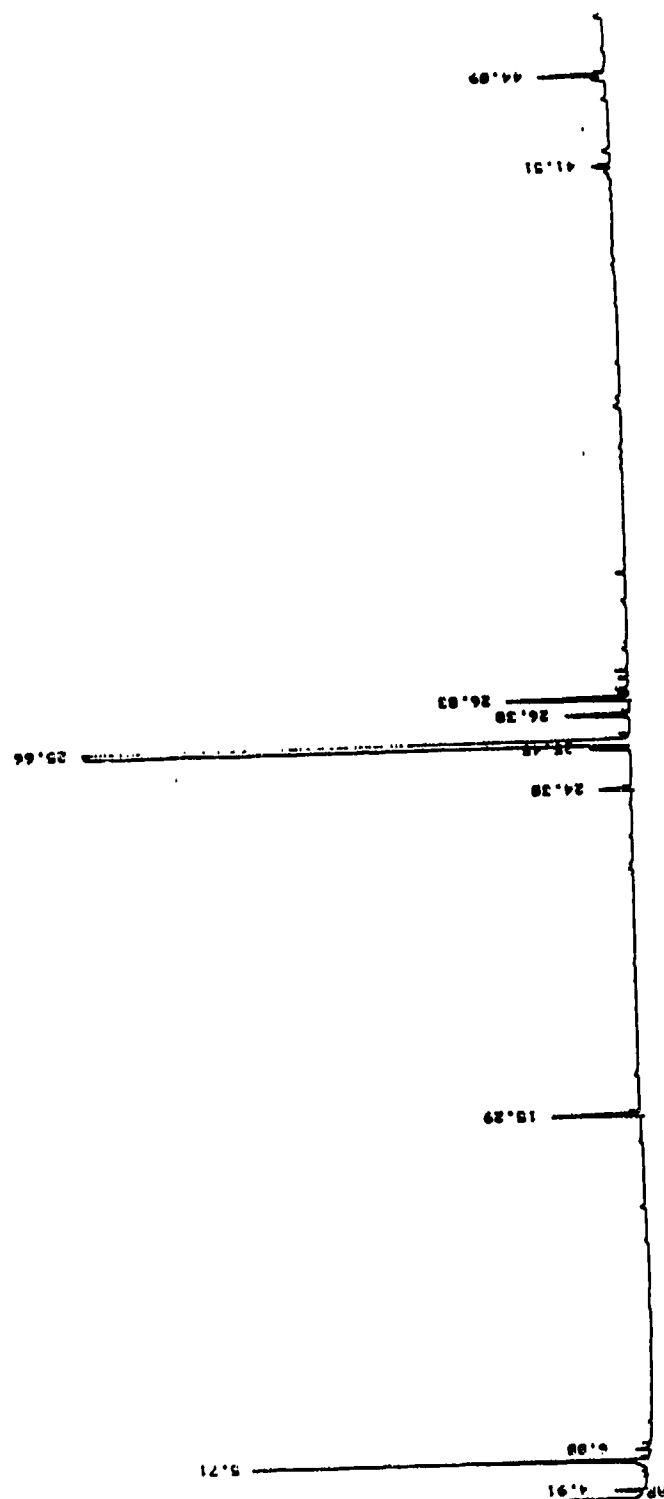
Figure 9. Splitless Injection GC Analysis of JP-10

from aqueous solutions by their Kovats indexes, and GC-MS analysis of each extract was not required.

Two types of GC-MS analyses were performed to identify the major fuel components of JP-4. The low boiling fraction (compounds eluting before n-nonane) was analyzed by an LKB GC-MS. A neat sample of the fuel was split during injection and was separated on a 40-m by 0.5-mm-ID OV-101 column. The components were identified by comparison with reference spectra (Stenhagen et al., 1974). For isomers that gave similar spectra, the boiling points were used to determine elution order. These identifications were confirmed by comparing the Kovats indexes with those compiled by Major Donald D. Potter, U.S. Air Force. Tables 5 through 7 list the major components of JP-4, JP-5, and JP-8.

The higher boiling fractions of the distillate fuels and all the high density fuels were dissolved in CS_2 and analyzed by the splitless injection technique on an SP-2100 fused silica capillary column. The mass spectrum of each peak was obtained on a Finnigan 3200 GC-MS.

The concentration of each component was calculated from the peak area determined from the GC analyses with FID. Since pure, authentic samples of each identified fuel component were not available, the total response factors for each peak were calculated in the following way. First, if the FID response factors are normalized to n-hexane = 1.00, then (with the exception of benzene and toluene) the detector response factors for aliphatic and low molecular weight aromatic hydrocarbons are proportional to the number of carbon atoms, within about $\pm$ 4% (Ettre, 1962). The detector response factor for benzene is 1.12 and toluene is 1.07. Therefore, it was assumed that the detector response factors for all compounds except benzene and toluene are 1.00. Second, the GC injector may be selective for compounds of low versus high boiling points. The total GC response factors were measured by preparing a solution of n-alkanes from n-heptane to n-octadecane and analyzing the solution by

TABLE 5. MAJOR COMPONENTS OF JP-4

Fuel Component	Kovats Index	Percent by Weight
n-Butane	400.0	0.12
Isobutane	466.3	0.66
n-Pentane	500.0	1.06
2,2-Dimethylbutane	527.7	0.10
2-Methylpentane	562.4	1.28
3-Methylpentane	578.7	0.89
n-Hexane	600.0	2.21
Methylcyclopentane	622.0	1.16
2,2-Dimethylpentane	629.1	0.25
Benzene	644.5	0.50
Cyclohexane	653.6	1.24
2-Methylhexane	669.5	2.35
3-Methylhexane	677.3	1.97
trans-1,3-Dimethylcyclopentane	679.6	0.36
cis-1,3-Dimethylcyclopentane	681.9	0.34
cis-1,2-Dimethylcyclopentane	684.4	0.54
n-Heptane	700.0	3.67
Methylcyclohexane	715.1	2.27
2,2,3,3-Tetramethylbutane	720.5	0.24
Ethylcyclopentane	729.8	0.26
2,5-Dimethylhexane	737.3	0.37
2,4-Dimethylhexane	738.4	0.58
1,2,4-Trimethylcyclopentane	740.8	0.25
3,3-Dimethylhexane	743.3	0.26
1,2,3-Trimethylcyclopentane	748.1	0.25
Toluene	753.0	1.33
2,2-Dimethylhexane	764.2	0.71
2-Methylheptane	772.0	2.70
4-Methylheptane	772.7	0.92
cis-1,3-Dimethylcyclohexane	775.3	0.42
3-Methylheptane	778.0	3.04
1-Methyl-3-ethylcyclohexane	784.1	0.17
1-Methyl-2-ethylcyclohexane	786.7	0.39
Dimethylcyclohexane	788.8	0.43
n-Octane	800.0	3.80
1,3,5-Trimethylcyclohexane	825.3	0.99
1,1,3-Trimethylcyclohexane	831.0	0.48
2,5-Dimethylheptane	833.6	0.52
Unidentified	839.9	0.98
Ethylbenzene	844.9	0.37
m-Xylene	853.9	0.96

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TABLE 5. MAJOR COMPONENTS OF JP-4 (CONCLUDED)

Fuel Component	Kovats Index	Percent by Weight
p-Xylene	854.8	0.35
3,4-Dimethylheptane	859.8	0.43
4-Ethylheptane	865.0	0.18
4-Methyloctane	868.5	0.86
2-Methyloctane	869.6	0.88
3-Methyloctane	873.9	0.79
o-Xylene	875.3	1.01
1-Methyl-4-ethylcyclohexane	881.3	0.48
n-Nonane	900.0	2.25
Isopropylbenzene	905.1	0.30
n-Propylbenzene	937.2	0.71
1-Methyl-3-ethylbenzene	944.9	0.49
1-Methyl-4-ethylbenzene	946.8	0.43
1,3,5-Trimethylbenzene	952.8	0.42
1-Methyl-2-ethylbenzene	961.0	0.23
1,2,4-Trimethylbenzene	975.6	1.01
n-Decane	1000.0	2.16
n-Butylcyclohexane	1025.6	0.70
1,3-Diethylbenzene	1031.4	0.46
1-Methyl-4-propylbenzene	1034.7	0.40
1,3-Dimethyl-5-ethylbenzene	1041.6	0.61
1-Methyl-2-i-propylbenzene	1049.1	0.29
1,4-Dimethyl-2-ethylbenzene	1060.2	0.70
1,2-Dimethyl-4-ethylbenzene	1067.1	0.77
n-Undecane	1100.0	2.32
1,2,3,4-Tetramethylbenzene	1128.8	0.75
Naphthalene	1156.5	0.50
2-Methylundecane	1156.0	0.64
n-Dodecane	1200.0	2.00
2,6-Dimethylundecane	1216.1	0.71
Unidentified	1262.3	0.68
2-Methylnaphthalene	1265.7	0.56
1-Methylnaphthalene	1276.4	0.78
n-Tridecane	1300.0	1.52
2,6-Dimethylnaphthalene	1379.4	0.25
n-Tetradecane	1400.0	0.73

TABLE 6.   MAJOR COMPONENTS OF JP-5

Fuel Component	Kovats Index	Percent by Weight
n-Octane	800.0	0.12
1,3,5-Trimethylcyclohexane	826.1	0.09
1,1,3-Trimethylcyclohexane	831.8	0.05
m-Xylene	854.4	0.13
3-Methyloctane	869.8	0.07
2,4,6-Trimethylheptane	874.4	0.09
o-Xylene	875.5	0.09
n-Nonane	900.0	0.38
1,2,4-Trimethylbenzene	975.7	0.37
n-Decane	1000.0	1.79
Unidentified	1015.9	0.61
n-Butylcyclohexane	1025.4	0.90
1,3-Diethylbenzene	1031.2	0.61
Unidentified	1037.5	0.50
1,4-Diethylbenzene	1041.3	0.77
4-Methyldecane	1060.3	0.78
2-Methyldecane	1063.1	0.61
1-Ethylpropylbenzene	1066.5	1.16
Unidentified	1083.9	0.54
Unidentified	1096.5	0.76
n-Undecane	1100.0	3.95
Unidentified	1112.8	0.78
2,6-Dimethyldecane	1119.1	0.72
1,2,3,4-Tetramethylbenzene	1128.3	1.48
Unidentified	1149.5	0.69
Naphthalene	1156.5	0.57
Unidentified	1157.5	0.51
Unidentified	1161.2	0.85
2-Methylundecane	1165.9	1.39
Unidentified	1186.8	0.83
n-Dodecane	1200.0	3.94
2,6-Dimethylundecane	1216.0	2.00
1,2,4-Triethylbenzene	1223.4	0.72
Unidentified	1229.7	0.56
Unidentified	1232.8	0.75
Unidentified	1249.6	0.56
Unidentified	1254.4	0.93
Unidentified	1256.1	0.61
Unidentified	1260.8	0.83
Unidentified	1261.8	0.65
2-Methylnaphthalene	1265.2	1.38
Unidentified	1271.2	0.90

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TABLE 6. MAJOR COMPONENTS OF JP-5 (CONCLUDED)

Fuel Component	Kovats Index	Percent by Weight
1-Methylnaphthalene	1275.8	1.44
Unidentified	1280.1	0.86
Unidentified	1285.0	0.70
1-Tridecene	1289.6	0.45
Phenylcyclohexane	1293.2	0.82
n-Tridecane	1300.0	3.45
1-t-Butyl-3,4,5-trimethylbenzene	1306.8	0.24
Unidentified	1316.9	0.67
Unidentified	1319.2	0.72
Unidentified	1323.6	0.53
Unidentified	1328.6	0.60
n-Heptylcyclohexane	1336.9	0.99
n-Heptylbenzene	1348.6	0.27
Biphenyl	1351.9	0.70
Unidentified	1359.8	1.18
Unidentified	1364.8	0.72
1-Ethylnaphthalene	1368.0	0.32
Unidentified	1371.2	0.74
2,6-Dimethylnaphthalene	1379.4	1.12
Unidentified	1385.7	0.58
Unidentified	1388.2	0.62
Unidentified	1393.7	0.53
n-Tetradecane	1400.0	2.72
Unidentified	1404.4	0.81
2,3-Dimethylnaphthalene	1410.4	0.46
Unidentified	1428.2	0.57
n-Octylbenzene	1450.0	0.78
Unidentified	1459.6	0.63
Unidentified	1465.4	1.02
Unidentified	1471.5	0.84
n-Pentadecane	1500.0	1.67
n-Hexadecane	1600.0	1.07
n-Heptadecane	1700.0	0.12

TABLE 7. MAJOR COMPONENTS OF JP-8

Fuel Component	Kovats Index	Percent by Weight
n-Heptane	700.0	0.03
n-Octane	800.0	0.09
1,3,5-Trimethylcyclohexane	825.9	0.06
1,1,3-Trimethylcyclohexane	831.9	0.06
m-Xylene	854.5	0.06
3-Methyloctane	870.0	0.04
2,4,6-Trimethylheptane	874.3	0.07
o-Xylene	875.7	0.06
cis-1-Ethyl-3-methylcyclohexane	881.9	0.10
n-Nonane	900.0	0.31
n-Propylcyclohexane	923.0	0.14
1,2,4-Trimethylbenzene	975.5	0.27
n-Decane	1000.0	1.31
n-Butylcyclohexane	1025.4	0.74
1,3-Dimethyl-5-ethylbenzene	1041.2	C.62
1,4-Dimethyl-2-ethylbenzene	1060.1	0.56
2-Methyldecane	1063.0	0.41
1-Ethylpropylbenzene	1066.4	0.99
Unidentified	1072.0	0.69
Unidentified	1096.5	0.79
n-Undecane	1100.0	4.13
Unidentified	1112.7	0.91
2,6-Dimethyldecane	1119.0	0.66
1,2,3,4-Tetramethylbenzene	1128.1	1.12
Unidentified	1130.1	0.88
Unidentified	1133.3	0.51
Unidentified	1149.3	0.98
Naphthalene	1155.9	1.14
Unidentified	1160.9	0.78
2-Methylundecane	1165.2	1.16
Unidentified	1171.1	0.77
Unidentified	1178.1	0.67
Unidentified	1186.3	1.12
Unidentified	1195.0	0.53
Unidentified	1200.0	4.72
n-Dodecane	1203.6	0.60
1,3,5-Triethylbenzene	1212.8	0.66
Unidentified	1215.7	2.06
2,6-Dimethylundecane	1222.7	0.99
1,2,4-Triethylbenzene	1229.3	0.59
Unidentified	1232.1	0.99
Unidentified	1236.6	0.93
n-Hexylcyclohexane		

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TABLE 7. MAJOR COMPONENTS OF JP-8 (CONCLUDED)

Fuel Component	Kovats Index	Percent by Weight
Unidentified	1248.6	0.66
Unidentified	1253.4	0.99
Unidentified	1255.4	0.56
Unidentified	1259.8	0.80
Unidentified	1261.1	0.55
2-Methylnaphthalene	1264.8	1.46
Unidentified	1270.5	0.85
1-Methylnaphthalene	1275.5	1.84
Unidentified	1279.1	0.86
Unidentified	1284.4	0.81
1-Tridecene	1289.3	0.73
Phenylcyclohexane	1292.6	0.37
n-Tridecane	1300.0	4.43
Unidentified	1316.2	0.66
Unidentified	1318.5	0.77
Unidentified	1323.0	0.53
Unidentified	1328.2	0.63
n-Heptylcyclohexane	1336.7	1.00
Unidentified	1340.4	0.56
n-Heptylbenzene	1347.7	0.25
Biphenyl	1351.3	0.63
Unidentified	1359.3	0.54
Unidentified	1364.3	0.67
1-Ethylnaphthalene	1367.2	0.33
Unidentified	1370.8	0.65
2,6-Dimethylnaphthalene	1378.9	1.34
Unidentified	1387.8	0.69
Unidentified	1393.0	0.69
n-Tetradecane	1400.0	2.99
Unidentified	1404.4	0.63
2,3-Dimethylnaphthalene	1410.4	0.36
n-Octylbenzene	1450.6	0.61
Unidentified	1465.6	1.02
Unidentified	1471.0	0.71
n-Pentadecane	1500.0	1.61
n-Hexadecane	1600.0	0.45
n-Heptadecane	1700.0	0.08
n-Octadecane	1800.0	0.02

capillary column GC. The peak areas were corrected for the actual weight
of the alkane and then normalized to n-octadecane = 1.00 to generate the
total response factors shown in Table 8. The average relative standard
deviation for three replicate analyses of the same solution was about
$\pm$ 2.5%. n-Octadecane was used as the internal standard for subsequent
analyses.

TABLE 8. RELATIVE RESPONSE OF THE CAPILLARY GC TO NORMAL ALKANES

Carbon Number	Relative Response[a]	Relative Standard Deviation[b]
7	0.93	1.4
8	1.03	2.8
9	1.07	2.5
10	1.07	2.1
11	1.07	2.0
12	1.05	2.3
13	1.06	2.5
14	1.06	2.6
15	1.02	2.5
16	1.04	2.5
17	1.03	2.8
18	1.00	2.7

[a] Normalized to n-octadecane

[b] Based on three replicate analyses of
the same solution.

The Finnigan GC-MS data system also can be used to record the ion
current for specific m/e values. This technique was used to identify the
molecular weights of the peaks in the high density fuels. These traces,
shown in Appendix C, (Figures C-4, C-5, and C-6), were used to assign the
molecular weights of the peaks listed in Table 9.

TABLE 9. MAJOR COMPONENTS OF THE HIGH DENSITY FUELS

Fuel and Components	Kovats Index	Molecular Weight ($g \, mole^{-1}$)	Percent by Weight
RJ-4			
Unidentified	1144.7	166,164	7.5
Unidentified	1149.7	164	7.4
Unidentified	1155.5	164	1.9
Unidentified	1173.2	164	2.4
Unidentified	1179.4	164	9.6
Unidentified	1185.5	164	10.6
Unidentified	1188.7	164	2.9
Unidentified	1193.2	164	20.7
Unidentified	1195.6	162	5.2
Unidentified	1200.0	164	8.7
Unidentified	1206.0	164	0.4
Unidentified	1208.2	164	1.8
Unidentified	1248.6	164,162	17.3
RJ-5			
Ethylbenzene	840.7	106	0.03
Xylenes	859.5,879.0	106	0.01
Unidentified	1443.6	184	0.34
Unidentified	1448.7	188	1.12
HXX	1464.9	186	2.03
Unidentified	1491.8	188	0.08
HNN	1510.4	186	96.32
Unidentified	1584.6	188	0.03
RJ-6			
XTHPCPD	1049.9	136	42.6
NTHDCPD	1079.4	136	1.1
Unidentified	1443.6	184	3.0
Unidentified	1448.7	188	7.1
Isomer I of RJ-5	1451.1	186	9.6
Unidentified	1464.9	186	11.2
Unidentified	1492.8	186	2.8
HNN	1509.3	186	20.2

TABLE 9.   MAJOR COMPONENTS OF THE HIGH DENSITY FUELS (CONCLUDED)

MAJOR COMPONENTS OF THE HIGH DENSITY FUELS (Concluded)

Fuel and Components	Kovats Index	Molecular Weight ($g\ mole^{-1}$)	Percent by Weight
JP-9			
n-Heptane	700.0	100	1.0
Methylcyclohexane	715.8	98	7.1
2,5-Dimethylhexane	728.1	128	0.8
Toluene	751.3	92	0.6
XTHDCPD	1049.6	136	66.8
NTHDCPD	1079.2	136	1.5
HNN	1509.6	186	20.1
JP-10			
XTHDCPD	1050.3	136	96.8
NTHDCPD	1079.6	136	1.5

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Professor Cornelius T. Moynihan of the Catholic University of America, Washington, D.C., kindly supplied authentic pure samples of several components of the high density fuels. His structural assignments and code abbreviations for these compounds are shown in Figure 10. No attempt was made to check his structural assignments.

3. FUEL-WATER PARTITIONING

The partitioning of the bulk fuels in deionized water or synthetic seawater was measured at a fuel:water ratio of 1:1000; the partitioning of JP-4, JP-8, and JP-9 was also measured at several other fuel:water ratios. The major experimental concerns in these studies were to be sure that no droplets of the fuel were present in the aqueous phase after equilibration and to minimize the rapid volatilization losses of the dissolved fuel components that may occur during handling of the aqueous solutions.

A solution of the water-soluble fuel component fraction was prepared at a fuel:water ratio of 1:1000 by injecting 100 µl of fuel from a syringe into 100 ml of water contained in a 150-ml centrifuge tube to disperse the fuel as tiny droplets in the water phase. The tube was sealed with a Teflon®-lined screw cap and gently mixed by rotation for 48 hours in a constant temperature bath. Following equilibration, the sample tubes were centrifuged for 30 minutes at 5000 rpm, which produced a relative centrifugal force of approximately 1500 g at the solution surface and 3500 g at the bottom of the tube. Then, the fuel was siphoned from the water's surface. A pipet was used to remove 5-ml aliquots of the remaining solution, which were immediately extracted with CS_2 containing a known amount of n-octadecane as an internal standard. Since the density of RJ-6 was slightly greater than the waters in which it was equilibrated, centrifugation caused the fuel to coalesce at the bottom of the vessel; the other fuels floated on the water's surface.

The fresh water used for the solubility measurements was deionized water from a Millipore water purification unit. Synthetic seawater was made from deionized water and the salts listed below. Blanks of both waters were routinely extracted and analyzed for possible interferences.

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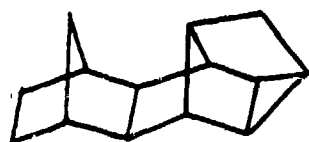
HXX

HXN
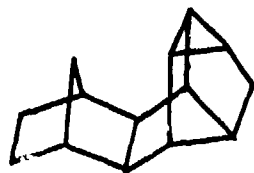
HNN
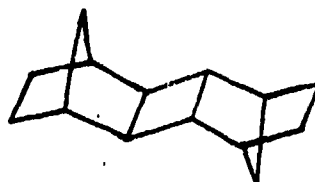
PXTX
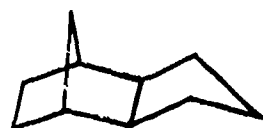
XTHDCPD

NTHDCPD

Figure 10. Structural Assignments of the High Density Fuel
Components Supplied by Professor Moynihan

| | Amount |
Salt	(g liter^{-1})
NaCl	23.96
$MgCl_2 \cdot 6H_2O$	10.63
Na_2SO_4	3.92
$CaCl_2 \cdot 2H_2O$	1.47
KCl	0.73
$NaHCO_3$	0.20

The major components in the fuels were identified by GC and GC-MS and quantified by GC, using the methods described in the previous section. The GC traces of the extracts of the fuels from deionized water are presented in Figures 11-18. Only a few of the fuel components have solubilities greater than 1 mg liter^{-1}. The solubilities of these fuels in seawater are similar to those in fresh water.

The solubilities of the major components of the fuels in deionized water and seawater are presented in Tables 10 through 13; complete data summaries for the distillate fuels may be found in Appendix C. All components of the high density fuels except XTHDCPD of JP-10 have very low solubilities. Minor aromatic impurities in these fuels were easily detected in the water-soluble fraction. The water-solvent blanks were carefully checked to assure that these aromatic compounds were indeed in the fuels.

As expected, the solubilities were generally lower in seawater than in deionized water at the same temperature. At a fuel:water ratio of 1:1000, the type of water has little effect on the partitioning. However, changing the fuel:water ratio from 1:10 to 1:10,000 at 20°C significantly reduced the concentration of the water soluble fractions of JP-4 and JP-8 and of the minor components of JP-9.

The following experiment was performed to determine the errors associated with the partitioning, extraction, and analysis steps of the

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Figure 11. GC Traces of JP-4 in CS_2
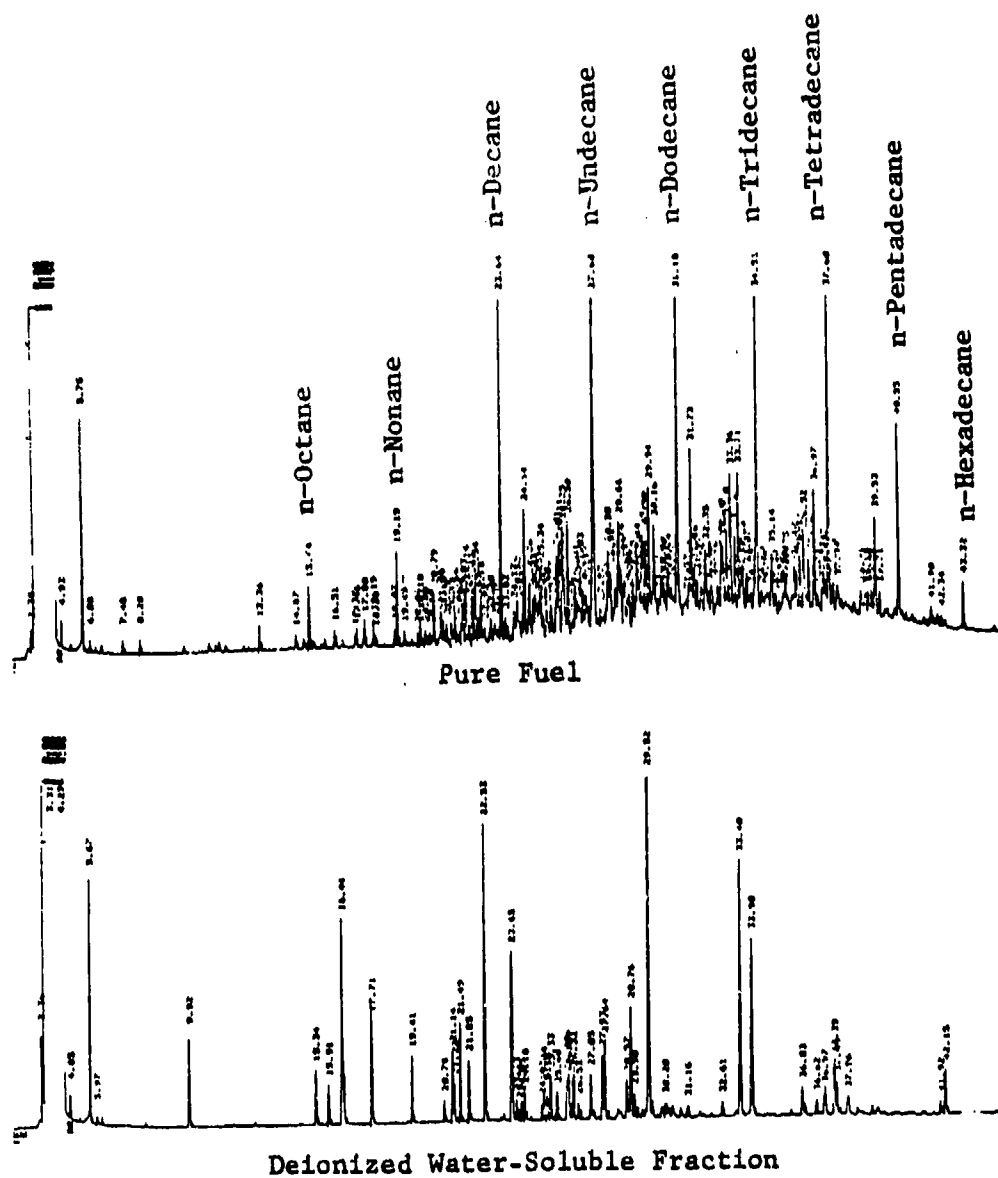
Figure 12. GC Traces of JP-5 in CS_2

Figure 13. GC Traces of JP-8 in CS_2

Pure Fuel

Deionized Water-Soluble Fraction
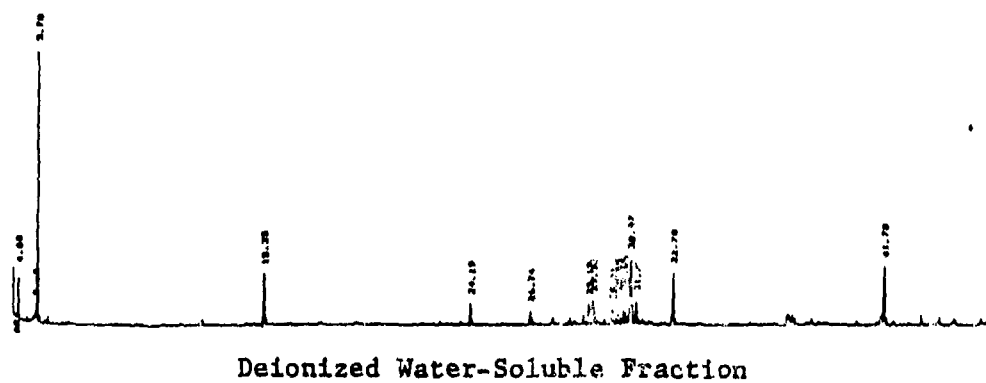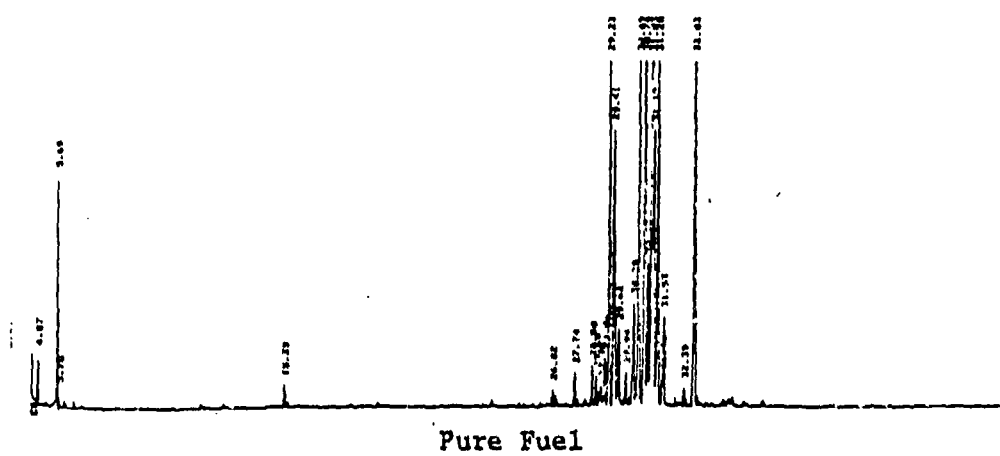
Figure 14. GC Traces of RJ-4 in CS_2
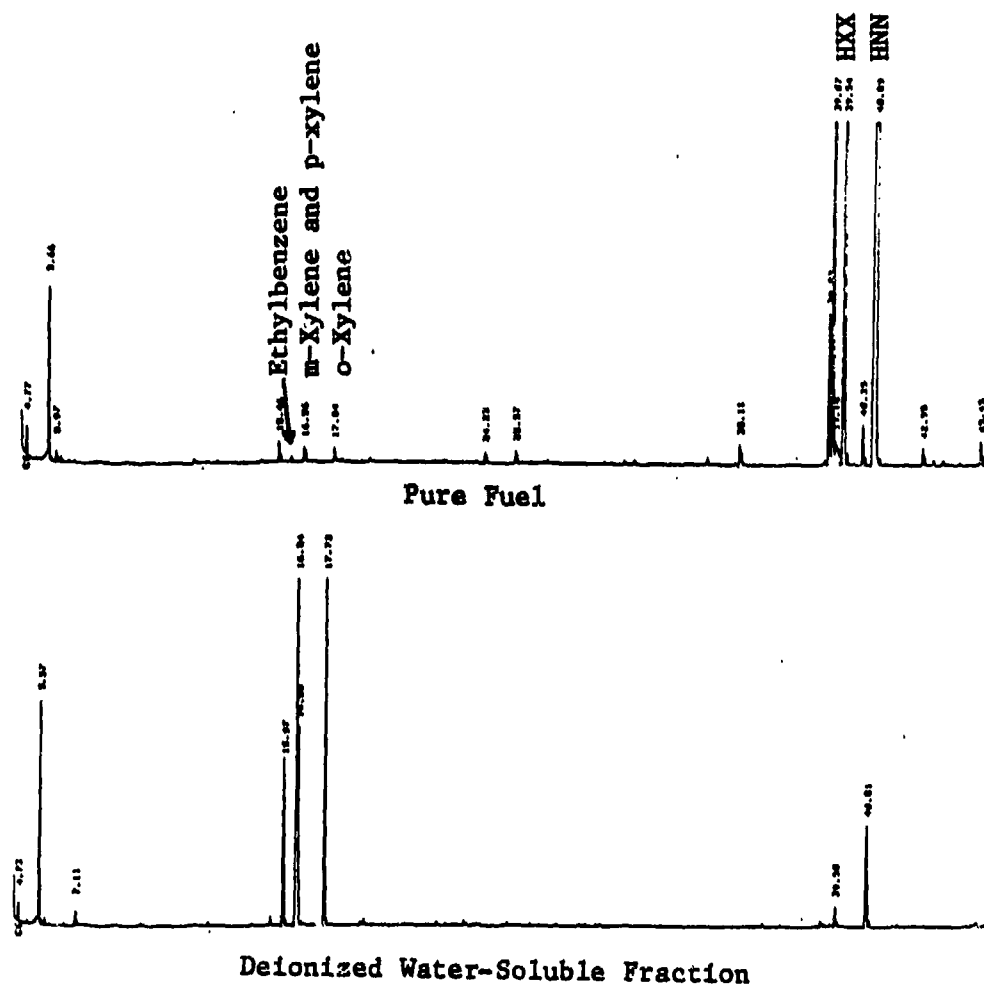
Figure 15. GC Traces of RJ-5 in CS_2
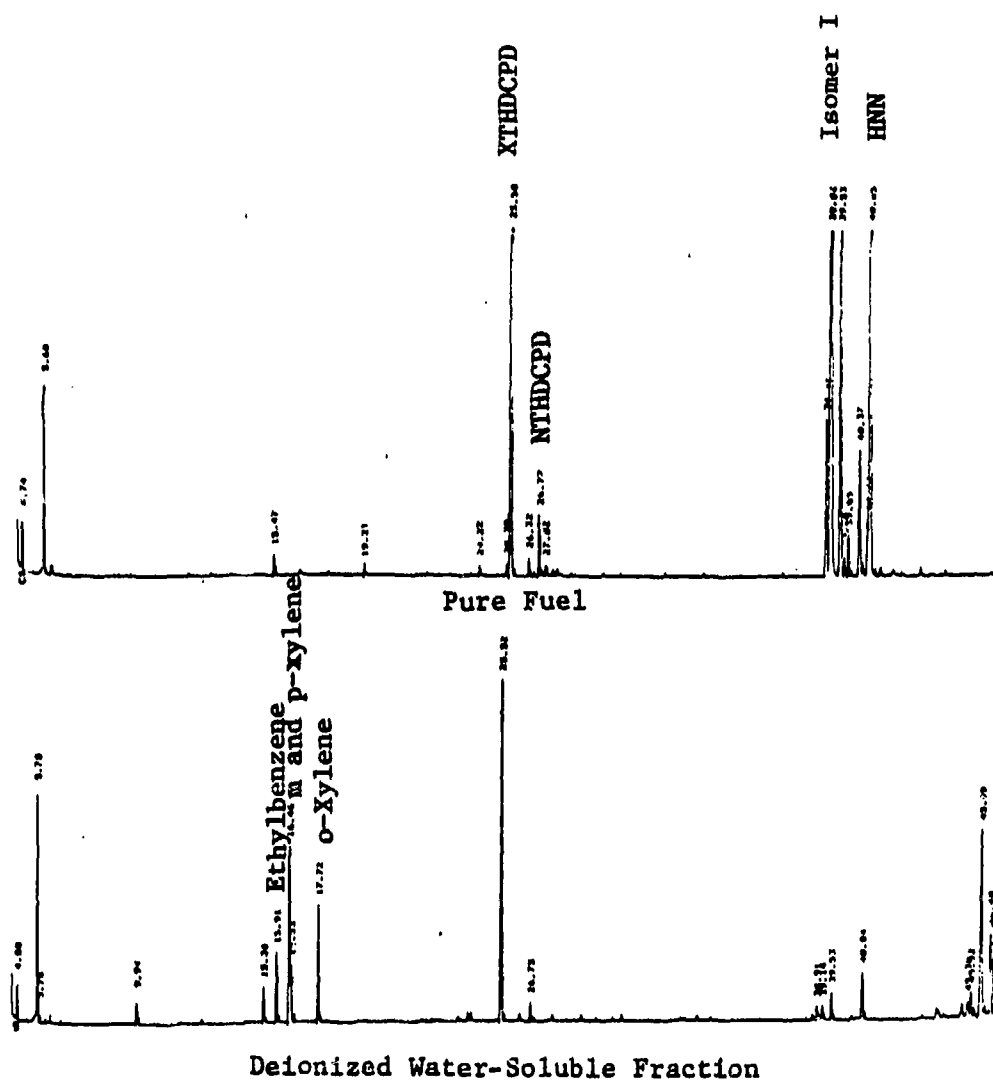
Figure 16. GC Traces of RJ-6 in CS$_2$

Figure 17. GC Traces of JP-9 in CS_2

Figure 18. GC Traces of JP-10 in CS_2

TABLE 10. CONCENTRATIONS OF THE MAJOR WATER-SOLUBLE COMPONENTS OF JP-4 AND JP-8 (mg liter^{-1})

Fuel-To-Water Ratio

Fuel Component	1:10		1:100		1:1000						1:10,000	
	Deion.[a] (20°C)	Sea.[b] (20°C)	Deion. (20°C)	Sea. (20°C)	Deion. (4°C)	Sea. (4°C)	Deion. (20°C)	Sea. (20°C)	Deion. (30°C)	Sea. (30°C)	Deion. (20°C)	Sea. (20°C)
JP-4												
Benzene	9.82	9.06	6.99	4.86	1.41	1.50	1.55	1.32	1.33	0.94	0.07	0.02
Cyclohexane	0.65	0.54	0.48	0.32	0.46	0.39	0.19	0.25	0.31	0.14	0.22	0.07
Toluene	8.49	7.09	7.79	4.95	3.78	3.50	3.71	3.00	3.23	2.64	0.70	0.50
Ethylbenzene	0.67	0.53	0.64	0.40	0.54	0.46	0.59	0.38	0.44	0.42	0.17	0.12
m-Xylene	2.01	1.41	1.83	1.10	} 1.97	1.30	1.89	1.06	1.28	1.22	0.55	0.35
p-Xylene	0.41	0.46	0.49	0.33		0.37	3.36	0.31	0.35	0.34	0.10	0.11
o-Xylene	1.21	0.95	1.17	0.74	0.91	0.79	1.08	0.67	0.78	0.78	0.27	0.21
1-Methyl-3-ethylbenzene	0.28	0.21	0.26	0.16	0.29	0.23	0.36	0.18	0.23	0.24	0.17	0.12
1,2,4-Trimethylbenzene	0.67	0.49	0.63	0.38	0.68	0.53	0.87	0.44	0.57	0.60	0.40	0.28
n-Decane	0.30	0.21	0.27	0.16	0.29	0.23	0.37	0.19	0.25	0.28	0.15	0.11
Naphthalene	0.39	0.29	0.31	0.22	0.27	0.22	0.41	0.24	0.30	0.32	0.10	0.08
2-Methylnaphthalene	0.16	0.11	0.11	0.05	0.12	0.09	0.19	0.10	0.17	0.15	0.10	0.06
1-Methylnaphthalene	0.08	0.06	0.06	0.05	0.08	0.06	0.13	0.06	0.11	0.10	0.06	0.04

[a] Deion. = deionized water.

[b] Sea. = artificial seawater.

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TABLE 10. CONCENTRATIONS OF THE MAJOR WATER-SOLUBLE COMPONENTS OF JP-4 AND JP-8 (mg liter^{-1}) (CONCLUDED)

Fuel Component	Fuel-to-Water Ratio													
	1:10		1:100		1:1000								1:10,000	
	Deion.^{a} (20°C)	Sea.^{b} (20°C)	Deion. (20°C)	Sea. (20°C)	Deion. (4°C)	Sea. (4°C)	Deion. (20°C)	Sea. (20°C)	Deion. (30°C)	Sea. (30°C)			Deion. (20°C)	Sea. (20°C)
JP-8														
Toluene	0.15	0.14	0.13	0.08	0.05	0.04	0.03	0.03	0.05	0.06			0.02	0.01
Ethylbenzene	0.05	0.04	0.04	0.03	0.03	0.02	0.02	0.01	0.03	0.02			0.01	<0.01
m-Xylene and p-xylene	0.15	0.12	0.13	0.09	0.09	0.07	0.07	0.04	0.08	0.06			0.03	0.02
o-Xylene	0.11*	0.09	0.10	0.07	0.06	0.05	0.05	0.03	0.06	0.05			0.01	0.01
1,2,4-Trimethylbenzene	0.20	0.16	0.18	0.11	0.16	0.11	0.15	0.08	0.15	0.10			0.07	0.06
n-Decane	0.15	0.12	0.13	0.08	0.12	0.09	0.12	0.06	0.11	0.08			0.05	0.04
1,2,3,4-Tetramethylbenzene	0.29	0.21	0.24	0.13	0.25	0.17	0.25	0.12	0.23	0.15			0.15	0.12
Naphthalene	0.41	0.34	0.31	0.22	0.25	0.19	0.31	0.20	0.28	0.22			0.06	0.06
2-Methylnaphthalene	0.34	0.27	0.17	0.10	0.15	0.11	0.19	0.11	0.18	0.13			0.08	0.06
1-Methylnaphthalene	0.15	0.12	0.12	0.08	0.13	0.09	0.16	0.10	0.15	0.11			0.07	0.05

^{a}Deion. = deionized water.

^{b}Sea. = artificial seawater.

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TABLE 11. CONCENTRATIONS OF THE MAJOR WATER-SOLUBLE COMPONENTS OF JP-5 (mg liter^{-1})

	Fuel-to-Water Ratio 1:1000	
Fuel Component	Deionized Water (20°C)	Artificial Seawater (20°C)
Toluene	0.06	0.03
Ethylbenzene	0.03	0.01
m-Xylene and p-xylene	0.16	0.09
o-Xylene	0.09	0.06
1-Methyl-3-ethylbenzene	0.05	0.03
1,2,4-Trimethylbenzene	0.20	0.12
n-Decane	0.14	0.08
Naphthalene	0.46	0.30
2-Methylnaphthalene	0.23	0.14
1-Methylnaphthalene	0.16	0.09

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TABLE 12. CONCENTRATIONS OF THE WATER-SOLUBLE COMPONENTS OF JP-9 (mg liter^{-1})

| | Fuel-To-Water Ratio | | | | | | | | | | | |
| Fuel Component | 1:10 | | 1:100 | | 1:1000 | | | | | | 1:10,000 | |
	Deion.[b] (20°C)	Sea.[c] (20°C)	Deion. (20°C)	Sea. (20°C)	Deion. (4°C)	Sea. (4°C)	Deion. (20°C)	Sea. (20°C)	Deion. (30°C)	Sea. (30°C)	Deion. (20°C)	Sea. (20°C)
n-Heptane	0.05	0.02	0.04	0.02	0.05	0.03	0.02	0.01	0.02	0.01	<0.01	<0.01
Methylcyclohexane	1.47	0.84	1.33	0.63	1.46	1.04	0.81	0.32	0.85	0.59	0.01	0.03
Dimethylhexane	0.13	0.07	0.13	0.06	0.13	0.09	0.07	0.03	0.08	0.05	<0.01	<0.01
Toluene	6.81	4.37	6.33	3.36	3.39	2.81	2.38	1.29	2.44	1.98	0.29	0.35
XTHDCPD	1.37	0.80	1.28	0.67	1.46	0.94	1.12	0.53	1.26	0.83	1.27	1.06
HNN	0.04	0.03	0.04	0.03	0.03	0.02	0.02	0.01	0.03	0.02	0.04	0.03

[b]Deion. = deionized water.

[c]Sea. = artificial seawater.

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TABLE 13. CONCENTRATIONS OF THE WATER-SOLUBLE COMPONENTS OF THE HIGH DENSITY FUELS

$$(\text{mg liter}^{-1})$$

Fuel and Components	Kovats Index	Fuel-to-Water Ratio 1:1000	
		Deionized Water (20°C)	Artificial Seawater (20°C)
RJ-4			
Unidentified	1144.7	0.01	<0.01
Unidentified	1149.7	0.01	<0.01
Unidentified	1179.1	0.01	<0.01
Unidentified	1185.3	0.01	<0.01
Unidentified	1193.2	0.04	0.01
Unidentified	1200.0	0.01	<0.01
Unidentified	1248.0	0.03	0.01
RJ-5			
Ethylbenzene	849.8	0.11	0.10
m-Xylene	859.0	0.32	0.30
p-Xylene	860.2	0.09	0.09
o-Xylene	879.3	0.23	0.21
HXX	1464.5	0.01	0.01
HNN	1508.9	0.07	0.07
RJ-6			
Ethylbenzene	850.2	0.05	0.05
m-Xylene	859.6	0.13	0.13
p-Xylene	860.5	0.03	0.04
o-Xylene	878.9	0.07	0.07
XTHDCPD	1049.2	0.32	0.54
NTHDCPD	1079.4	0.01	0.01
HNN	1508.9	0.03	0.02
JP-10			
Ethylbenzene	850.2	0.02	0.02
m-Xylene and p-xylene	860.1	0.11	0.09
o-Xylene	879.5	0.02	0.02
XTHDCPD	1049.4	1.49	0.96
NTHDCPD	1079.1	0.03	0.02

partitioning studies. Two identical samples of JP-4 were partitioned with deionized water. Two aliquots of the aqueous fraction were extracted from each tube, and each extract was analyzed twice. The raw data are presented in Appendix C, Table C-4. A standard computer program (SAS Institute, Inc., Cary, NC) was used to estimate the contribution to variation in the concentration of the nine components in the water due to the sample, extraction, and GC analysis steps.

The results presented in Table 14 are interesting in that the total error is only about ±5% of the mean of the eight samples, regardless of the concentration of the component. However, the percent of the error explained by the sample and extraction clearly depends on the component's concentration.

4. VOLATILIZATION STUDIES

The volatilization rates of the major water-soluble fuel components in JP-4, JP-8, and JP-9 were measured from water equilibrated with the fuel at a 1:1000 fuel:water ratio. All the fuel components except naphthalene and its derivatives were expected to be high volatility compounds (Smith et al , 1980, and Section III.4.). Therefore, the gas phase mass transport coefficients were not measured.

The volatilization measurement procedures described in the literature and in Section III.4 were followed. The fuels were equilibrated with deionized water described in Section IV.3. The fuel-saturated water from six equilibration tubes was combined in a 600-ml beaker to give a 500-ml sample. The solution was transfered to the beaker by pipet with a minimum of turbulence to minimize volatilization of the fuel components before sampling. A constant speed propeller-type stirrer was used to stir the solution. During the experiment, 5-ml samples were removed at appropriate time intervals and immediately extracted with CS_2 containing n-octadecane as an internal standard. The extracts were then analyzed by capillary column GC. The volatilization rate constants were calculated for each compound using equation (18).

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TABLE 14. ERROR ANALYSIS FOR WATER-SOLUBLE FRACTION

| Fuel Component | Percent of Error Explained by: | | | Mean Concentration (ppm) | Coefficient of Variation |
	Sample	Extraction	Analysis		
Benzene	26.9	34.6	38.5	0.79	7.1%
Cyclohexane	87.9	3.0	9.1	0.15	8.3
Toluene	0.0	76.5	23.5	2.37	4.5
m + p-Xylene	0.0	74.3	27.8	1.43	4.6
o-Xylene	0.0	73.5	26.5	0.68	4.6
1-Methyl-3-ethylbenzene	24.7	61.2	14.1	0.22	3.8
1,2,4-Trimethylbenzene	26.9	52.6	20.5	0.55	4.8
n-Decane	63.2	24.5	12.3	0.24	4.7
Naphthalene	33.9	55.4	10.7	0.25	3.7
Average	29.3	50.6	20.3		
Standard deviation	30.0	25.2	9.7		

Following collection of the last sample, N_2 was introduced to purge
the solution of oxygen. Without changing the stirring rate, the rate of
solution reaeration was monitored with a dissolved oxygen analyzer. The
oxygen reaeration rate constant was then calculated from equation (29).

The values for k_v^C/k_v^O are summarized in Tables 15 and 16. All the
water-soluble fuel components are high volatility compounds ($k_v^C/k_v^O \approx 0.52$)
except for naphthalene and its derivatives. The concentration of the
norbonadiene dimers (RJ-5 isomers) in water was so low that volatilization
rate measurements were not possible.

5.   PHOTOLYSIS OF JP-4

The influence of exposure to direct sunlight on the water-soluble
components of JP-4 was studied in deionized water, a natural fresh water,
and a natural salt water. Before equilibration with the fuel, the two
natural waters were centrifuged and filtered to remove suspended particles
and microbes. Aqueous solutions of JP-4 were prepared from 1:1000
fuel:water mixtures as previously described. The water solutions were
then transfered by pipet to quartz photolysis tubes, and the tubes were
sealed. Care was taken to avoid a head space or the trapping of air
bubbles, which could allow fuel component volatilization during the
experiment.

The photolysis tubes were placed on the roof on a rack along with a
second identical series of tubes wrapped with foil to exclude light.
These served as the dark control samples. After 7, 14, and 21 days of
light exposure, one light exposed and one dark control tube for each of
the three waters were removed for sampling. A 5-ml sample was removed
from each tube and immediately extracted with CS_2 containing n-octadecane
as an internal standard. The extracted samples were analyzed by capillary
column GC.

The data are summarized in Table 17 and C-7 and Figure 19. The
loss of naphthalene and the substituted naphthalenes can be explained by
direct photolysis. The losses of the alkylated benzenes, however, must
be rationalized by an indirect photolysis process. The reasons are des-
cribed below.

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TABLE 15. VOLATILIZATION RATE DATA FOR THE MAJOR WATER-SOLUBLE COMPONENTS OF JP-4 AND JP-8

Fuel Component	JP-4 k_v^C/k_v^0				JP-8 k_v^C/k_v^0			
	$k_v^0 = 2.81$ hr^{-1}	$k_v^0 = 5.82$ hr^{-1}	$k_v^0 = 15.1$ hr^{-1}	Average k_v^C/k_v^0	$k_v^0 = 2.71$ hr^{-1}	$k_v^0 = 4.33$ hr^{-1}	$k_v^0 = 17.0$ hr^{-1}	Average k_v^C/k_v^0
Benzene	0.52	0.32	0.30	0.38 ± 0.12	—	—	—	—
Cyclohexane	0.65	0.50	0.55	0.57 ± 0.08	—	—	—	—
Toluene	0.64	0.50	0.80	0.65 ± 0.15	0.37	0.74	—	0.56 ± 0.26
Ethylbenzene	0.64	0.51	0.56	0.57 ± 0.07	—	—	—	—
m-Xylene and p-xylene	0.61	0.48	0.86	0.65 ± 0.19	0.28	0.76	0.82	0.62 ± 0.30
o-Xylene	0.58	0.46	0.73	0.59 ± 0.14	0.29	0.75	0.51	0.52 ± 0.23
1-Methyl-3-ethylbenzene	0.60	0.49	0.54	0.54 ± 0.06	0.35	0.68	—	0.52 ± 0.23
1,2,4-Trimethylbenzene	0.57	0.45	0.74	0.59 ± 0.15	0.26	0.62	0.48	0.45 ± 0.18
n-Decane	0.56	0.43	0.46	0.48 ± 0.07	0.26	0.59	0.48	0.44 ± 0.17
1,2,3,4-Tetramethylbenzene	0.54	0.42	0.46	0.47 ± 0.06	0.24	0.47	0.44	0.38 ± 0.13
Naphthalene	0.30	0.24	0.51	0.35 ± 0.14	0.22	0.28	0.20	0.23 ± 0.04
2-Methylnaphthalene	0.32	0.26	0.58	0.39 ± 0.17	0.22	0.32	0.25	0.26 ± 0.05
1-Methylnaphthalene	0.27	0.21	0.25	0.24 ± 0.03	0.21	0.25	0.20	0.22 ± 0.03

TABLE 16. VOLATILIZATION RATE DATA FOR THE MAJOR WATER-SOLUBLE COMPONENTS OF JP-9

	k_v^C/k_v^O			Average
Fuel Component [a]	$k_v^O = 2.87 \ hr^{-1}$	$k_v^O = 5.91 \ hr^{-1}$	$k_v^O = 13.7 \ hr^{-1}$	k_v^C/k_v^O
Methylcyclohexane	0.41	0.38	0.66	0.48 ± 0.15
2,5-Dimethylhexane	0.73	0.44	0.51	0.56 ± 0.15
Toluene	0.43	0.39	0.57	0.46 ± 0.69
XTHDCPD	0.38	0.36	0.43	0.39 ± 0.04

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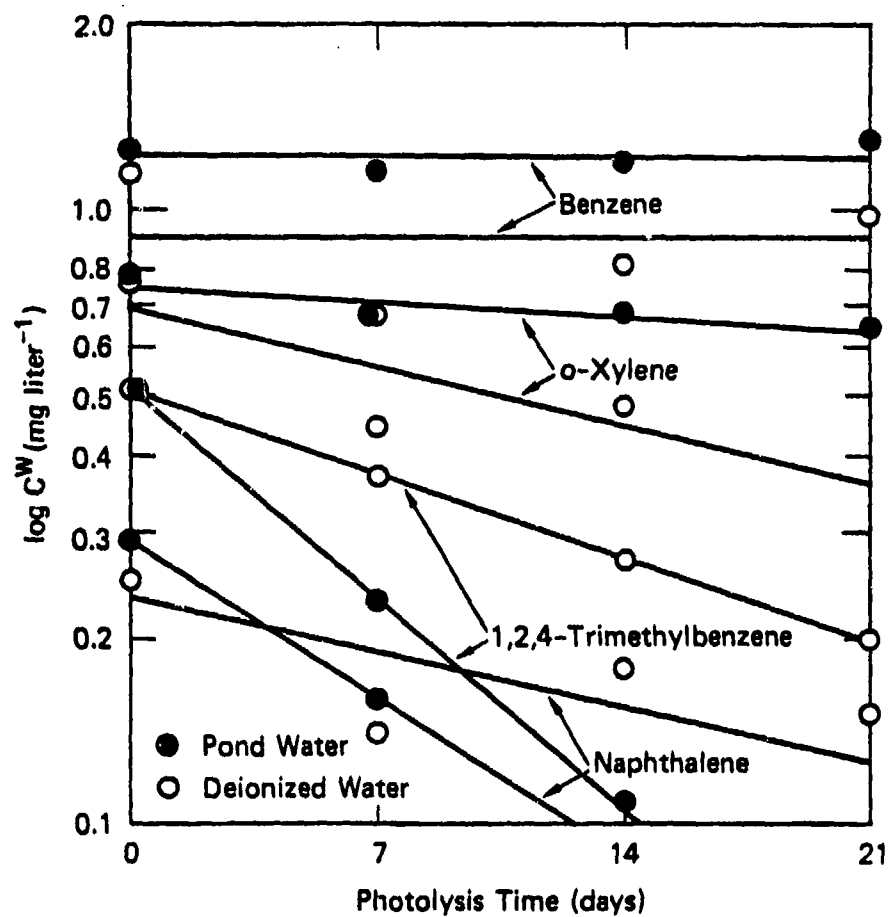
Figure 19. Photolysis of Selected Aromatic Water-Soluble Fuel Components of JP-4.

TABLE 17. PHOTOLYSIS OF THE MAJOR WATER-SOLUBLE FUEL COMPONENTS OF JP-4 IN WATER

Fuel Component Concentration (mg liter^{-1})

Fuel Component	Deionized Water				Artificial Seawater				Pond Water			
	Control*	7 Days	14 Days	21 Days	Control	7 Days	14 Days	21 Days	Control	7 Days	14 Days	21 Days
Benzene	1.15	0.68	0.82	0.98	0.76	0.88	0.67	0.65	1.24	1.16	1.20	1.32
Cyclohexane	0.23	0.15	0.17	0.26	0.10	0.11	0.09	0.08	0.31	0.28	0.34	0.34
Toluene	2.82	1.75	1.95	2.01	2.22	2.61	2.07	1.95	2.86	2.74	2.80	2.85
Ethylbenzene	0.40	0.25	0.27 *	0.25	0.36	0.42	0.33	0.30	0.40	0.40	0.41	0.40
m-Xylene and p-xylene	1.43	0.87	0.85	0.63	1.30	1.54	1.15	0.99	1.46	1.38	1.34	1.20
o-Xylene	0.74	0.45	0.48	0.37	0.70	0.79	0.63	0.58	0.75	0.68	0.68	0.65
1-Methyl-3-ethylbenzene and 1-Methyl-4-ethylbenzene	0.29	0.16	0.14	0.08	0.27	0.32	0.22	0.18	0.28	0.27	0.27	0.22
1,2,4-Trimethylbenzene	0.51	0.23	0.11	0.01	0.49	0.31	0.05	--	0.52	0.37	0.19	0.10
n-Decane	0.23	0.13	0.09	0.03	0.23	0.23	0.15	0.10	0.24	0.19	0.18	0.14
Naphthalene	0.25	0.14	0.18	0.15	0.26	0.06	<0.01	--	0.29	0.16	0.09	0.01
2-Methylnaphthalene	0.10	0.04	0.05	0.02	0.10	<0.01	<0.01	--	0.11	0.03	0.02	--
1-Methylnaphthalene	0.07	0.03	0.04	0.01	0.07	<0.01	<0.01	--	0.08	0.03	0.02	--

*Average of 7, 14 and 21 day dark control samples.

Direct photolysis occurs when a chemical absorbs light and then undergoes reaction from an electronic excited state. The rate constant for direct photolysis is given by

$$k_p = \phi b \Sigma \, \epsilon_\lambda I_\lambda \tag{34}$$

where ϕ is the reaction quantum yield, b is a unit conversion constant, ϵ_λ is the absorption coefficient of the chemical, and I_λ is the light flux (or irradiance) of sunlight for the specific wavelength interval, λ.

Naphthalene absorbs light between 290 and 330 nm, and the quantum yield for direct photolysis of naphthalene in pure water is 1.5×10^{-2} (Mabey et al., 1981). The direct photolysis rate constant for naphthalene can be calculated using the ϵ_λ and I_λ values in Mabey et al (1981a) and the procedures described in Mabey et al (1981b). The values, which are averaged over a 24-hour day, have been calculated for the four seasons. The calculated k_p value for naphthalene in July is 0.08 day^{-1}, which corresponds to a half-life of 9 days. The half-life for spring (or April) was not calculated, but it is slightly longer than the summer half-life. These calculations are in accord with the measured half-lives of naphthalene in the water-soluble fraction of JP-4 where half-lives in natural and pure water during May-June are from 8 to 20 days.

Direct photolysis of benzene or alkylated benzenes is not expected to be significant because their ϵ_λ values above the solar cutoff wavelength (~290 μm) are very small. One explanation for the loss of alkylated benzenes is that trace amounts of oxidation products in the pure fuel may be extracted into the water during preparation of the aqueous solutions because they contain polar oxygen functional groups. If carbonyl-containing species are present, the loss of the alkylated benzene during photolysis can be explained by the following process.

Mill (1981) has pointed out that the rate constant for abstraction of hydrogen by alkoxy radicals (I) is similar to that of the triplet excited state carbonyls(II)

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$$RO\cdot + H-\overset{|}{\underset{|}{C}}- \rightarrow \cdot\overset{|}{\underset{|}{C}}- + ROH$$
$$I$$

$$\rangle C=O + h\nu \xrightarrow[\text{crossing}]{\text{intersystem}} \rangle\dot{C} - \dot{O}$$
$$II$$

$$\rangle\dot{C}-\dot{O} + H-\overset{|}{\underset{|}{C}}- \rightarrow -\overset{}{\underset{/}{C}} + \rangle\dot{C}-O-H$$
$$II$$
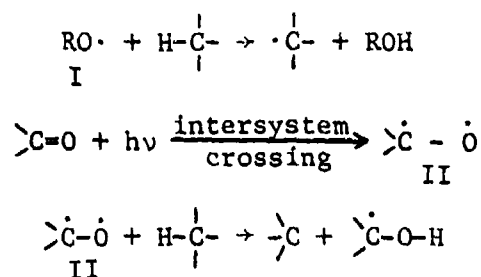
and that the triplet state oxy radicals may be formed in sunlit aquatic systems when carbonyl-containing compounds are present. The triplet state oxy radicals may then oxidize alkylated benzene by removal of the benzylic hydrogen. For o-xylene, the following reaction applies
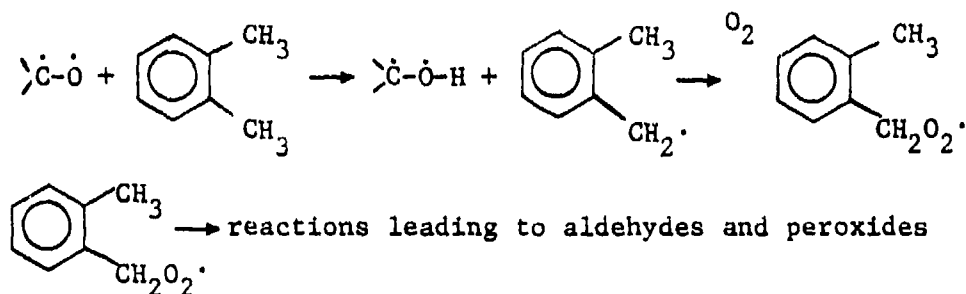
Formation of aldehydes and peroxides would then propagate the free radical oxidation of xylene and other chemicals containing benzylic hydrogen.

To determine the feasibility of this suggested mechanism, the data were evaluated as follows. Mill (1981) has reported that the rate constant, k_{ox}, for oxidation of benzylic hydrogen by alkoxyl radical is 10^6 M^{-1} s^{-1} per hydrogen. The first-order rate constants k_m measured for the loss of o-xylene and 1,2,4-trimethylbenzene are between 7×10^{-8} and 1.4×10^{-6} s^{-1} (these rate constants were calculated for the slowest and fastest reactions in Figure 19). If the statistical corrections for the number of benzylic hydrogens on the alkylated benzenes are ignored and a middle value for k_m of 1×10^{-6} is assumed, a 24-hour averaged steady-state concentration of 10^{-12} M alkoxyl radical can be calculated from the simple kinetic expression.

$$k_m = k_{ox} [OX] \tag{35}$$

where [OX] is the concentration of the alkoxyl radical or triplet carbonyl

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species.   Although this calculation is probably good only within several
orders of magnitude and contains many simplifications and assumptions,
it does show that only a low concentration of the free radical process-
initiating species need be present; the carbonyl-containing components
would not be detected using the analytical procedures.

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SECTION IV

DISCUSSION AND CONCLUSIONS

Three subjects will be discussed in this section:

- Partitioning of the fuel components in the environment.
- Estimates of the volatilization rates of the water-soluble fuel components from water to air.
- The significance of other environmental fate processes that should be considered in evaluating the effects of a fuel spill.

1. PARTITIONING OF THE FUEL COMPONENTS IN THE ENVIRONMENT

The fuel-water partitioning data and the distillate and high density fuels were summarized in Section IV.3 and Tables 10 through 13. The major water-soluble components are the aromatics. This is most strikingly seen in the water-soluble components of the high density fuels, where minor aromatic components of the fuels were selectively partitioned into the water.

From the concepts of fugacity and the octanol-water partition coefficient, K_{oc}, (Equation 11) described in Section III.3a, it seemed reasonable to predict that a similar concept, the fuel-water partition coefficient, K_{fw}, could be developed from the data in Tables 11 through 13. where

$$K_{fw} = C_f/C_w \tag{36}$$

Table 18 presents the logarithms of the solubility and K_{fw} of the fuel components for those compounds for which both reliable aqueous solubility and fuel and water concentrations were available. The values of $-\log S$ and $\log K_{fw}$ are plotted in Figure 20. The slope and intercept of the data were calculated using a linear least squares analysis. The results at a fuel:water ratio 1:1000 are as follows:

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TABLE 18. SOLUBILITY AND FUEL-WATER PARTITION COEFFICIENTS (K_{fw}) IN DEIONIZED WATER (FUEL:WATER = 1:1000).

Fuel Component	$-\log S^a$ (mol liter^{-1})	JP-4 log K_{fw}	JP-5 log K_{fw}	JP-8 log K_{fw}
Methylcyclopentane	3.30	4.97	--	--
Benzene	1.65	3.39	--	--
Cyclohexane	3.07	4.69	--	--
2-Methylhexane	4.60	5.57	--	--
3-Methylhexane	4.58	5.56	--	--
n-Heptane	4.64	5.50	--	--
Methylcyclohexane	3.79	4.87	--	--
Toluene	2.22	3.44	--	--
n-Octane	5.42	5.98	--	--
Ethylbenzene	2.91	3.68	--	--
m-Xylene	2.90	3.57	3.83	3.89
p-Xylene	2.83	3.88	--	--
o-Xylene	2.80	3.85	4.01	4.15
1,2,4-Trimethylbenzene	3.36	3.95	4.17	4.17
i-Propylbenzene	3.34[b]	4.25	4.26	4.38
Naphthalene	3.61	3.88	4.00	4.47
2-Methylnaphthalene	3.75[b]	4.35	4.68	4.80
1-Methylnaphthalene	3.71[b]	4.67	4.85	4.96

[a] S = solubility of the component in water at 20°C in mol liter^{-1}.

[b] Lande and Banerjee (1981)

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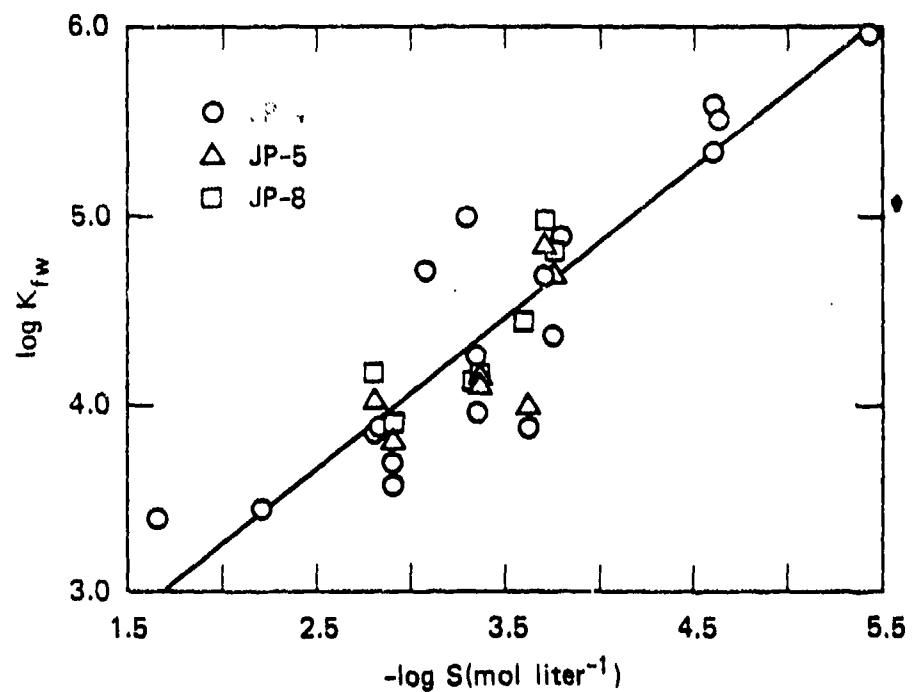
JA-1614-7

Figure 20. Aqueous Solubility of the Pure Distillate Fuel Component (S) as a
Function of the Fuel-Water Partition Coefficient (K_{fw})
(Fuel:water = 1:1000, 20°C).

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- JP-4

$$\log K_{fw} = -0.797 \log S + 1.681, \quad r^2 = 0.82 \tag{37}$$

- JP-5

$$\log K_{fw} = -0.746 \log S + 1.757, \quad r^2 = 0.57 \tag{38}$$

- JP-8

$$\log K_{fw} = -0.864 \log S + 1.508, \quad r^2 = \quad \tag{39}$$

- All Fuels

$$\log K_{fw} = -0.799 \log S + 1.664, \quad r^2 = 0.79 \tag{40}$$

A similar correlation for the high density fuels should be possible if solubility data for the individual components were available. Correlation equations for fresh and salt water at each temperature and each fuel-to-water ratio could also be developed.

The correlation equations can be used to predict the concentration of a fuel component in water, provided the concentration of the component in the fuel is known, using equation (36). For instance, the values for toluene in JP-4 are $\log S = -2.22$, $\log K_{fw} = -3.44$, and $C_f = 1.33\% = 0.0133 \times 761.6 = 10.1$ g liter^{-1}. Then

$$\log K_{fw} = 0.797 \times 2.22 + 1.681 = 3.450$$
$$K_{fw} = 2820 \text{ (measured value} = 2750)$$
$$C_f = 10.1/2820$$
$$= 3.59 \times 10^{-3} \text{ g liter}^{-1} \text{ (measured value} = 3.71 \times 10^{-3} \text{ liter}^{-1})$$

Mackay and Patterson (1981) described a simple procedure for calculating the equilibrium distribution of a chemical in the environment. The procedure is based on estimating the fugacity coefficient (Section III.3a and Equations 10 and 12) for the chemical and the size and physical properties of the environment. Mackay's environmental parameters are summarized below.

$$T = 20°C = 293 \text{ K}$$
$$\text{Air:} \quad V = 10^{10} \text{ m}^3$$
$$\text{Soil:} \quad V = 9 \times 10^3 \text{ m}^3$$
$$\rho_s = 1.5 \text{ g cm}^{-3}$$
$$f_{oc} = 0.02$$

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Water: $V = 7 \times 10^6 \text{ m}^3$

Biota: $V = 3.5 \text{ m}^3$

$\rho_b = 1.0 \text{ g cm}^{-3}$

Suspended solids: $V = 35 \text{ m}^3$

$\rho_s = 1.5 \text{ g cm}^{-3}$

$f_{oc} = 0.04$

Sediment: $V = 2.1 \times 10^4 \text{ m}^3$

$\rho_s = 1.5 \text{ g cm}^{-3}$

$f_{oc} = 0.04$

The procedure used to calculate the environmental distributions is described by Mackay and Patterson (1981) in great detail and is not repeated here. The method was applied to five representative fuel components, n-pentane, n-decane, benzene, ethylbenzene, and naphthalene, which represent th range of the major fuel components of the distillate fuels. Table 19 summarizes the values of constants such as K_{oc} and K_b for each component, the fugacity coefficients z_i, the predicted concentrations in the six phases (assuming a total of 100 moles of the component is in the environment), and the percentage of the total amount in each phase.

The results show that the alkane fuel components will equilibrate almost entirely in the air, but the aromatics may be in the air and water (benzene, ethylbenzene) or the water and sediments (naphthalene). All the alkane fuel components should behave like pentane and decane. The other monoaromatics, toluene, xy es, and C_3-substituted benzenes, should behave much like benzene and ethylbenzene, while the substitued naphthalenes should behave like naphthalene. As the degree of substitution on the aromatic ring increases, the percentage found in the sediments will increase. The C_4- and higher substituted monoaromatics may behave more like naphthalene because their solubility in water decreases as the degree of substitution increases.

Note that this analysis does not predict the rate of transport between phases, nor does it address the rate of transformation in the phases. This is di cussed in the next subsection.

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TABLE 19. MACKAY'S LEVEL 1 ENVIRONMENTAL DISTRIBUTION OF REPRESENTATIVE DISTILLATE FUEL COMPONENTS[a].

	n-Pentane	n-Decane	Benzene	Ethylbenzene	Naphthalene
Aqueous solubility ($g\ m^{-3}$)	39.0	5.14^{b}	1760	141	31.4
$H(P_a\ m^3\ mol^{-1})^c$	126	1200	0.61	0.86	0.049
$z^a = 1/RT$ ($mol\ m^{-3} P_a^{-1}$)	4.1×10^{-4}	4.1×10^{-4}	4.1×10^{-4}	4.1×10^{-4}	4.1×10^{-4}
$z^w = 1/H$ ($mol\ m^{-3} P_a^{-1}$)	7.9×10^{-3}	8.3×10^{-4}	1.6	1.2	20
K_{oc}^d	1600	2.0×10^4	51	600	1000
K_p (soil)^e	32	400	1.0	12	20
K_p (sediments)^f	64	800	2.0	24	40
$z^s = K_p \rho_s/H$ (soil)	0.38	0.50	2.5	21	610
$z^s = K_p \rho_s/H$ (sediment)	0.76	1.0	5.0	42	1200
K_b^g	200	2000	8.2	91	120
$z^b = K_b \rho_b/H$	1.6	1.7	13	110	2400
Concentrations($mol\ m^{-3}$)^h					
Air	9.8×10^{-9}	9.9×10^{-9}	2.5×10^{-9}	2.9×10^{-9}	1.9×10^{-10}
Soil	9.1×10^{-6}	1.2×10^{-5}	1.5×10^{-5}	1.5×10^{-4}	2.9×10^{-4}
Water	1.9×10^{-7}	2.0×10^{-8}	9.9×10^{-6}	8.4×10^{-6}	9.4×10^{-6}
Biota	3.8×10^{-5}	4.1×10^{-5}	8.0×10^{-5}	7.7×10^{-4}	1.1×10^{-3}
Suspended sediments	1.8×10^{-5}	8.5×10^{-4}	1.1×10^{-3}	2.9×10^{-4}	5.7×10^{-4}
Sediments	1.8×10^{-5}	8.5×10^{-4}	1.1×10^{-3}	2.9×10^{-4}	5.7×10^{-4}
Percentage of Total					
Air	98.2%	99.2%	25.3%	28.7%	1.9%
Soil	0.1	0.1	0.1	1.3	2.6
Water	1.3	0.1	74.0	63.8	70.8
Biota	0.0	0.0	0.0	0.0	0.0
Suspended sediments	0.0	0.0	0.0	0.0	0.0
Sediments	0.4	0.5	0.6	6.2	24.6

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[a] Assumes that T = 293°K, soil and sediment density = ρ_s = 1.5 g cm^{-3}, and biota density = ρ_b = 1.0g cm^{-3}. Procedure is taken from Mackay and Patterson (1981).

[b] The solubility was estimated from the vapor pressure and Henry's constant, using Equation 24.

[c] Table 3. $H(P_a\ m^3\ mol^{-1})$ = H(unitless) $\times$ 5.47 $\times 10^{-5}$

[d] $\log K_{oc}$ = -0.921 $\log X_s$ -0.00953(mp-25°C) - 1.405 (see Karickhoff, 1981, for details)

[e] K_p = 0.02 K_{oc} (soils)

[f] K_p = 0.04 K_{oc} (sediments and suspended sediments)

[g] $\log K_b$ = 2.066 - 0.85 $\log C_s$ (mol m^{-3})

[h] Assuming that the total amount of chemical in the environment is 100 moles.

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2. PREDICTED ENVIRONMENTAL FATE OF THE WATER-SOLUBLE FUEL COMPONENTS

Tables 15 and 16 summarize the values of k_v^C/k_v^O for the water-soluble fuel components. If the values for naphthalene and the methylnaphthalenes are omitted, the average value of k_v^C/k_v^O for all the major fuel components is 0.515 with a standard deviation of 0.087. This suggests that all the alkanes, cycloalkanes, and monoaromatics are high volatility compounds in the distillate and high density fuels, meaning that liquid phase mass transport resistance determines the volatilization rate.

The average value of k_v^C/k_v^O, Equation (31), and the $(k_v^O)_{env}$ data in Table 4 were used to estimate the environmental half-lives of the water-soluble fuel components. The results of the calculations, summarized in Table 20, suggest that the environmental half-lives of the water-soluble fuel components excluding naphthalene and its derivatives.

TABLE 20. VOLITIZATION HALF-LIVES FOR THE
HIGH-VOLATILITY WATER-SOLUBLE FUEL COMPONENTS.

	k_v^C (hr^{-1})	Half-Life (hr)	(days)
Pond	4.1×10^{-3}	170	7.1
River	2.1×10^{-2}	34	1.4
Lake	5.2×10^{-3}	140	5.8

The value of k_v^C/k_v^O for three fuel components, naphthalene, and 1- and 2-methylnaphthalene, are about 0.2 to 0.4, which is significantly less than the values for the more volatile compounds. Smith et al (1981) made extensive studies of the volatilization rate of naphthalene and found that the volatilization rate is determined by both gas and liquid phase mass transport resistance. This means that both terms of Equation (23) are important. Smith et al (1981) showed the the following expression can be used to predict the volatilization rate of naphthalene.

$$k_v^C = \frac{1}{L}\left[\frac{1}{k_\ell^O\left(D_\ell^C/D_\ell^O\right)} + \frac{1}{H\,k_g^W\left(D_g^C/D_g^W\right)}\right]^{-1} \qquad (41)$$

where D is the diffusion constant in water or air of the chemical, oxygen, or water, and k_g^W is the gas phase mass transport coefficient for water. Values of the various constants for naphthalene are recommended by Smith et al.

$$D_\ell^C/D_\ell^O = 0.35$$
$$k_\ell^O = k_v^C/L \ \ (k_v^C \text{ from Table 4})$$
$$H = 0.020 \ \text{(Table 3)}$$
$$k_g^W = 2100 \text{ cm hr}^{-1}$$
$$D_g^C/D_g^W = 0.28$$

These data are used in Equation (39) to predict the half-lives of naphthalene as follows:

Pond: $t_{\frac{1}{2}} = 260$ hr

River: $t_{\frac{1}{2}} = 67$ hr

Lake: $t_{\frac{1}{2}} = 230$ hr

Values of H for 1- and 2-methylnaphthalene were not available, but their half-lives should be slightly longer than naphthalene.

These volatilization half-lives can be compared with the photolysis data summarized in Table 17. Benzene and the water soluble non-aromatic components of both the distillate and the high density fuels will not undergo chemical transformation processes. Therefore, volatilization from water to air should be the dominant environmental fate of these fuel components. Photolysis of these compounds in air may be reasonably fast.

Naphthalene and alkylated benzenes will undergo direct photolysis and photooxidation, respectively, in aqueous fuel solutions. Naphthalene will have a photolysis half-life of at least a week during the summer and longer half-lives during other seasons or in cloudy weather. In aquatic

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systems, the alkylated benzenes will photolyze more slowly than in our experiments because the carbonyl species, which we assume to be responsible for the photooxidations, will be more diluted by the larger volume of the receiving water. Mill (1981) has estimated that concentrations of alkoxyl radicals (including triplet carbonyl species) may be on the order of 10^{-14} M in aquatic systems. Therefore, we conclude that loss of alkylated benzenes in the environment will be at least two orders of magnitude slower than in our experimental work; the photolysis half-lives would then be at least several years. Thus, photolysis will not be an important environmental fate for any of the water-soluble fuel components except naphthalene and the substituted naphthalenes.

Little is known about the importance of other major fate processes of the water-soluble fuel components, biodegradation and adsorption. Both of these processes will be studied in other Air Force research programs. However, the data in Table 19 suggest that adsorption of naphthalene and its isomers may be significant.

3. RECOMMENDATIONS FOR FURTHER RESEARCH

The concept of developing fuel-water partitioning coefficients, which should be useful procedure for estimating the aqueous concentration of a fuel component after a spill, deserves further study. The correlation would be improved if the solubilities of more of the substituted benzenes were available. Additional work on the analytical methods for extracting and concentrating the water-soluble fraction would improve the accuracy and precision of the partitioning data.

We believe that two major fate processes have not received adequate attention: the rate of dissolution of the water-soluble fuel components and the rate of evaporation of the pure fuels. There is considerable evidence that a major fate of a spilled hydrocarbon fuel is evaporation into the atmosphere, where the fuel vapors are rapidly diluted and photolyzed. In a search of Chemical Abstracts, we could find no studies of the evaporation or dissolution rate of jet fuels, kerosene, or gasoline. However, Regnier and Scott (1975) studied the loss of

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n-alkanes from a No. 2 fuel oil. Mackay and Matsugu (1973) and Harrison
et al (1975) studied the rate of evaporation of crude oil components from
an oil slick. Several references were found on the dissolution rates of
hydrocarbon components in seawater (McAuliffe et al , 1980; Greene et al ,
1977). If volatilization of the fuel components directly from the spilled
fuel to the air is faster than the rate of dissolution, the importance
of the aquatic processes (volatilization, biodegration, photolysis, and
adsorption) will be diminished considerably. There is also evidence
that the fuel components may be photolyzed in the pure fuel slick (Larson
et al , 1977). Research on all these processes is clearly needed.

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Appendix A

FUEL ANALYSIS BY STANDARD METHODS

TABLE A-1. PHYSICAL PROPERTIES OF JP-4

Sample __Fuel 1A GEC-145-400-792033 (JP-4)__

Viscosity (cSt) MRC	-30°F (SFQLA)	2.46
	-20°F	2.206
	32°F	1.288
	70°F	0.9546
	100°F	0.7864
Surface Tension (dyne/cm) MRC	-20°F	27.52 *extrapolated
	32°F	25.05
	70°F	23.28
	100°F	21.73
Density (g/CC) MRC	-20°F	0.7957
	32°F	0.7957
	70°F	0.7557
	100°F	0.7423
Gravity (60/60) D287/Calo SFQLA		54.3 °API 0.7616 Specific
Freezing Pt. SFQLA		-64 °C -83 °F

TABLE A-1. PHYSICAL PROPERTIES OF JP-4 (CONTINUED)

Sample   <u>Fuel 1A GEC-145-400-792033 (JP-4)</u>

Color D156	+20
Acidity (mg KOH/g) D3242	0.002
Copper Strip (2 hrs at 212°F) D130	1A
Existent Gum (mg/100 ml) D381	0.8
Particulates (mg/1) D2276	0.1
Filtration Time D2276	17 min @ 27"
Water Reaction, Vol. Change (ml) D1094	0.0
Ratings D1094	#1 #1
WSIM, Minisonic	96

Additives

1. Anti-icing (Vol %)   07
2. Antioxidant (lb/M Bbl)
3. Corrosion Inhibitor (lb/M Bbl)
4. Metal Deactivator (lb/M Bbl)
5. Antistatic (ppm)

TABLE A-1. PHYSICAL PROPERTIES OF JP-4 (CONTINUED)

Sample ___Fuel 1A GEC-145-400-792033 (JP-4)___

79-F-2270
79-F-245
45
45A
09

Composition

	Vol %	
	Mass spec MRC	SFQLA
1. Paraffins	61.2	
2. Monocycloparaffins	24.2	
3. Dicycloparaffins	4.9	
4. Alkylbenzenes	8.2	
5. Indans and Tetralins	1.1	
6. Indenes and Dihydronaphthalenes	---	
7. Naphthalenes	0.4	
Aromatics (4 + 5 + 6 + 7) D1319	9.7	12.3
Olefins D1319		1.5
Total Paraffins (1+2+3)/D1319(100%-A-O)	90.3	86.2

Hydrogen Content (wt %) POSF - 03701 / SFQLA - D3343	14.48	14.46
Sulfur, Mercaptan (wt %) D1219-61		0.0004
Total (wt %) D2622-67		0.03
Net Heat of Combustion (BTU/lb) (MRC-D240/SFQLA-D3338)	18767	18747
Luminometer Number D1740		77.
Smoke Pt. (SFQLA-Calc/SFQLA-D1322)	28	25.0

TABLE A-1. PHYSICAL PROPERTIES OF JP-4 (CONCLUDED)

FUEL VOLATILITY

Sample **FUEL 1A GEC-145-400-792033 (JP-4)**

Vol % Recovered	JP-4	JP-8	SFOLA 2887 °C	MRC 2887 °C	SFOLA D86 °C	D86 °F	
IBP (0.5%)	*	+	28	25	60	140	IBP
1				34			
5			72	72			
10	*	++	89	93	97	206	10
15			97				
20	**	+	104	108	110	230	20
25			115				
30			119	123	___	___	30
35			126				
40			137	141	___	___	40
45			144				
50	**	+	155	160	146	295	50
55			166				
60			176	180	___	___	60
65		•	188		•		
70			197	199	___	___	70
75			208				
80			217	218	___	___	80
85			228				
90	**	+	237	237	224	435	90
95			253	254			
99				273			
FBP (99.5%)	**	++	283	281	248	478	FBP
Residue (%)	**	++				1.0	
Loss (%)	**	++				1.0	
Recovery at 400°F (%) (204.4°C)						82.0	
Vapor Pressure (lb Reid)	**				2.5		

Flash pt (°C)	++	D56 (Tag Closed)	D93 (Pensky-Martens)	D3243 (Setaflash)	
True Vapor Pressure		-20°F	+32°F	+70°F	100°F

TABLE A-2. PHYSICAL PROPERTIES OF JP-5

TEST METHOD	APPEARANCE	RESULTS	SPEC LIMIT	REPORT DATE COMPLETED
11 D156	Color (Saybolt)	− 9		9 May 1980
20	Visual (H=Bright and C=Clear)			CONTRACT NO.
	COMPOSITION			ORDER NO.
100 D974	Acidity, Total (mg KOH/g)	. 0 0 2		80-F-607
110 D1319	Aromatics (vol %)	1 6 . 1		DATE SAMPLED
120 D1319	Olefins (vol %)	0 . 9		RECD 28 Apr 80
130 D1219	Sulfur, Mercaptan (wt %)	. 0 0 0 1 4		SAMPLE NO.
140 D484	Doctor Test (propm, negative)			DDP-80-18
150 D1266	Sulfur, Total (wt %)	. 1 0		BATCH NO.
	VOLATILITY		D-86	
200 D86	Distillation Initial BP (C) ASTM D-2887	1 2 2	IBP 351	
205	10% Rec (C)	1 7 9	10 385	TANK NO.
210	20% Rec (C)	1 9 4	20 398	(F-1)
215	50% Rec (C)	2 2 2 .	30 407	QUANTITY U.S. GALLONS
220	90% Rec (C)	2 6 2	40 416	
225	95% Rec (C)	2 7 0	50 426	SAMPLING LOCATION
230	Final BP (C)	2 9 1	60 436	Major D. Potter
235	Residue (%)	.	70 447	AFWAL/POSF
240	Loss (%)	.	80 460	
245	Recovery at 400 F (%)	.	90 478	PRODUCT NAME
250 FTMS1151	Explosiveness (vol %)		EP 511	
260 D56	Flash Point (F)		RES 1.0	COMPLIES WITH SPECIFICATION
270 D287	Gravity, API (60 F)	4 2 . 6	LOSS 1.0	
280 D1289	Gravity, Specific (60/60 F)	. 8 1 2 8		
290 D323	Vapor Pressure (lb Reid)	.		
	FLUIDITY			RSA LABORATORY
300 D2386	Freezing Point (F)	− 5 2		Det 13 SA-ALC/SFQLA
310 D455	Viscosity at -30 F (cSt)	1 1 . 9		Aerospace Fuels Lab
	COMBUSTION			WPAFB OH 45433
400 D1405	Aniline-Gravity Product			GRADE
410 D1405	Net Heat of Combustion (Btu/lb) CALC	1 8 5 8 5		(JP-5)
420 D1740	Luminometer Number	5 3		REMARKS
430 D1322	Smoke Point CALC 22	2 3 . 0		
440 D1840	Napthalenes (vol %)	.		Fuel tested as per
XXX	HYDROGEN WT %	1 3 . 8 1		request. No Remarks.
	CORROSION			
500 D130	Copper Strip (2 h at 212F)	1 A		
510 IP227	Silver Strip			
	STABILITY			
600 D1660	Coker Δ P (in. Hg)	.		
610 D1660	Coker Tube Color Code			
	CONTAMINANTS			
700 IP225	Copper Content (µg/kg)			
710 D381	Existent Gum (mg/100 ml)	1 . 0		
720 D2276	Particulates (mg/liter)	1 . 1		1x5 Gal Can
730 D1094	Water Reaction Vol Change (ml)	0 0 . 0		
740 D1094	Water Reaction Ratings	1 b 2		
750 D2550	WSIM M.S.	5 0		
	ADDITIVES BRAND			
800	Antiicing (vol %)	. 1 0		
810	Antioxidant (lb/M Bbl)	.		
820	Corrosion Inhibitor (lb/M Bbl)	.		
830	Metal Deactivator (lb/M Bbl)	.		
840	Antistatic, ppm	.		
	OTHER TESTS			
900 D2624	Conductivity (CU)			
	FILTRATION TIME 10 MIN @26"			

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APPROVED
THOMAS J. O'SHAUGHNESSY
Chief, Aerospace Fuels Laboratory
Directorate of Energy Management

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TABLE A-2. PHYSICAL PROPERTIES OF JP-5 (CONCLUDED)

RUN TIMES/WIDTH 41.94   .00   10

BASE LEVELS   2.43   2.42

RUN   25   SIMULATED DISTILLATION   23 APR 30

INST   1   SD METHOD 142   FILE   42   0:

% OFF	TIME	TEMP
IBP	12.57	122.1
5	16.76	167.6
10	17.87	179.2
15	18.67	187.4
20	19.34	194.2
25	19.71	198.0
30	20.27	203.6
35	20.80	208.9
40	21.31	214.2
45	21.66	217.6
50	22.13	222.4
55	22.66	227.8
60	23.07	232.0
65	23.46	235.9
70	23.95	240.8
75	24.51	246.4
80	25.02	251.5
85	25.46	255.8
90	26.18	262.8
95	26.92	270.0
FBP	29.07	291.4

80-1-807
80-634-M

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TABLE A-3. PHYSICAL PROPERTIES OF JP-8

Sample ____FUEL 2A GEC-140-800-792033 (JP-8)____

Viscosity (cSt) MRC	-30°F (SFQLA)	_____
	-20°F	9.101
	32°F	3.526
	70°F	2.233
	100°F	1.665
Surface Tension (dyne/cm) MRC	-20°F	31.17* extrapolated
	32°F	28.78
	70°F	27.08
	100°F	25.69
Density (g/CC) MRC	-20°F	0.8460
	32°F	0.8252
	70°F	0.8096
	100°F	0.7977

Gravity (60/60) D287/Calc   __42.3__ °API __0.8142__ Specific
   SFQLA

Freezing Pt.   __-8__ ° C   __-47__ °F
   SFQLA

TABLE A-3.   PHYSICAL PROPERTIES OF JP-8 (CONTINUED)

Sample   FUEL 2A GEC-140-800-792033 (JP-8)

Color D156	+20
Acidity (mg KOH/g) D3242	0.002
Copper Strip (2 hrs at 212°F) D130	1A
Existent Gum (mg/100 ml) D381	0.0
Particulates (mg/1) D2276	0.5
Filtration Time D2276	11 min @ 27"
Water Reaction, Vol. Change (ml) D1094	0.0
Ratings D1094	#1 #1
WSIM, Minisonic	65

Additives

1. Anti-icing (Vol %)   0.14

2. Antioxidant (lb/M Bbl)

3. Corrosion Inhibitor (lb/M Bbl)

4. Metal Deactivator (lb/M Bbl)

5. Antistatic (ppm)

TABLE A-3. PHYSICAL PROPERTIES OF JP-8 (CONTINUED)

Sample ___FUEL 2A GEC-140-800-792033 (JP-8)___ 79-F-227

245

Composition

45

45

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		Vol %	
		Mass spec MRC	SFQLA
1.	Paraffins	44.4	
2.	Monocycloparaffins	41.4	
3.	Dicycloparaffins	2.6	
4.	Alkylbenzenes	6.7	
5.	Indans and Tetralins	3.4	
6.	Indenes and Dihydronaphthalenes	–	
7.	Naphthalenes	1.5	
	Aromatics (4 + 5 + 6 + 7) D1319	11.6	16.8
	Olefins D1319		2.1
	Total Paraffins (1+2+3)/D1319(100%-A-0)	88.4	81.1

	MRC	SFQLA
Hydrogen Content (wt %) POSF - D3701 / SFQLA - D3343	13.94	13.78
Sulfur, Mercaptan (wt %) D1219-61		0.0004
Total (wt %) D2622-67		0.11
Net Heat of Combustion (BTU/lb) (MRC-D240/SFQLA-D3338)	18576	18591
Luminometer No. ···er D1740		48
Smoke Pt. (SFQLA-Calc/SFQLA-D1322)	22	26.0

TABLE A-3. PHYSICAL PROPERTIES OF JP-8 (CONCLUDED)

FUEL VOLATILITY

Sample: FUEL 2A GEC-140-800-792033 (JP-8)

Vol % Recovered	JP-4	JP-8	SFOLA 2887 °C	MRC 2887 °C	SFOLA D86 °C	D86 °F	
IBP (0.5%)	*	♦	144	128	183	361	IBP
1				144			
5			175	176			
10	*	♦♦	188	190	202	396	10
15			195				
20	**	♦	200	203	208	406	20
25			205				
30			210	214			30
35			215				
40			218	222			40
45			221				
50	**	♦	226	231	221	429	50
55			230				
60			234				60
65			237				
70			242	249			70
75			248				
80			253	259			80
85			251				
90	**	♦	264	272	248	478	90
95			272	282			
99				300			
FBP (99.5%)	**	♦♦	296	306	267	512	FBP
Residue (%)	**	♦♦				1.0	
Loss (%)	**	♦♦				1.0	
Recovery at 400°F (%) (204.4°C)							
Vapor Pressure (lb Reid)	**						
Flash pt (°C)		♦♦	D56 (Tag Closed)	D93 (Pensky-Martens) 54	D3243 (Setaflash)		
True Vapor Pressure			-70°F	+32°F	+70°F	100°F	

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TABLE A-4. PHYSICAL PROPERTIES OF RJ-4

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TEST METHOD	APPEARANCE	RESULTS	SPEC LIMIT	Report Info
D.56	Color (Saybolt)			**REPORT DATE COMPLETED** 8 May 1980
55	Visual (B) Bright and (C) Clear			**CONTRACT NO.**
COMPOSITION				
100 D974	Acidity Total (mg KOH g)	•		EXXXXXX 80-F-605
115 D1319	Aromatics (vol %)	•		**DATE SAMPLED**
11 D1319	Olefins (vol %)	•		RECD 28 Apr 80
13 D3227	Sulfur Mercaptan (wt %)	•		**SAMPLE NO.** DDP 80-12
140 D484	Doctor Test (Pos/Neg)			**BATCH NO.** Lot 0109
150 D1266	Sulfur Total (wt %)	• 0 2		**TANK NO.**
VOLATILITY				
200 D86	Distillation Initial BP (F)	4 0 8		
205	10% Rec (F)	2 1 1		
210	30% Rec (F)	4 1 2		
215	50% Rec (F)	4 1 4		**QUANTITY U.S. GALLONS**
220	90% Rec (F)	4 2 0		
225	95% Rec (F)			**SAMPLING LOCATION** Major D. Potter AFWAL/POSF
230	Final BP (F)	4 6 3		
235	Residue (%)	1 • 0		
240	Loss (%)	1 • 0		
245	Recovery at 400 F (%)	•		**PRODUCT NAME**
255 FTMS 1151	Explosiveness (vol %)			
260 D56	Flash Point (F)	1 6 6	SPECIFIC 0.9230	**COMPLIES WITH SPECIFICATION**
275 D287	Gravity API 60 F	2 1 • 8		
285 D1298	Gravity Specific (60/60 F)	• 9 2 3 0		
290 D323	Vapor Pressure (lb Reid)	•		
FLUIDITY				
300 D2386	Freezing Point (F)	-		**LABORATORY** Det 13 SA-ALC/SFQLA Aerospace Fuels Lab WPAFB OH 45433
310 D455	Viscosity at XXF (cSt) 0°F	1 7 • 5		
COMBUSTION				
400 D1405	Aniline-Gravity Product		BTU GAL	**GRADE** RJ-4
410 D1405	Net Heat of Combustion (Btu/lb)	1 8 3 9 2	141,360	**REMARKS**
420 D1740	Luminometer Number			
430 D1322	Smoke Point	•		
440 D1840	Naphthalenes (vol %)	•		Fuel Tested as per request.
450 D1655	Smoke Volatility Index	•		
CORROSION				
500 D130	Copper Strip (2 h at 212F)			
510 IP227	Silver Strip			
STABILITY				
600 D1660	Coker & P (in. Hg)	•		
610 D1660	Coker Tube Color Code			
CONTAMINANTS				
700 IP225	Copper Content (ug/kg)			
710 D381	Existent Gum (mg/100 ml)	0 • 6		
720 D2276	Particulates (mg/liter)	•		
730 D1094	Water Reaction Vol Change (ml)	•		1 x 1 Gal Can
740 D1094	Water Reaction Ratings			
750 D2550	WSIM			
ADDITIVES / BRAND				
800	Antiicing (vol %)	•		
810	Antioxidant (lb/M bbl)	•		
820	Corrosion Inhibitor (lb/M bbl)	•		
830	Metal Deactivator (lb/M bbl)	•		
840	Antistatic, ppm	•		
OTHER TESTS				
900 D2624	Conductivity (CU)			

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Directorate of Energy Management

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TABLE A-5. PHYSICAL PROPERTIES OF RJ-5

TEL	METHOD	APPEARANCE	RESULTS	SPEC LIMIT	REPORT DATE Completed
10	D156	Color (Saybolt)	+ 2 9		27 Oct 78
20		Visual (H=Bright and C=Clear)		RED NOV 06 1978 RVN	CONTRACT NO. 78-D-0023
		COMPOSITION			
100	D974	Acidity, Total (mg KOH/g)	.	RED NOV 06 1978	78-F-2292
110	D1319	Aromatics (vol %)	.		
120	D1319	Olefins (vol %)	.		DATE SAMPLED 25 Oct 78
130	D1219	Sulfur, Mercaptan (wt %)	. 0 0 0 0		Rec'd 26 Oct 78
140	D484	Doctor Test (p=pos, n=negative)			SAMPLE NO. 78-17
150	D1266	Sulfur, Total (wt %)	. 0 2		
		VOLATILITY			BATCH NO. 8285
200	D86	Distillation Initial BP (F)	4 8 0		
205		10% Rec (F)	5 1 2		TANK NO. 6
210		20% Rec (F)	5 1 3		
215		50% Rec (F)	5 1 5		QUANTITY U.S. GALLONS 1250
220		90% Rec (F)	5 1 8		
225		95% Rec (F)			SAMPLING LOCATION Ashland Chemical Co. 5200 Blazer Parkway Dublin OH 53017
230		Final BP (F)	5 5 0		
231		Residue (%)	1 . 0		
240		Loss (%)	1 . 0		
245		Recovery at 400 F (%)	.		PRODUCT NAME Propellant Fuel
250	TMS1151	Explosiveness (vol %)			
260	L156	Flash Point (F)	2 2 4 SetaFlash 226°F		COMPLIES WITH SPECIFICATION
270	D187	Gravity, API (60 F)	.		
280	D1209	Gravity, Specific (60/60 F)	1 . 0 8 9 0		MIL-T-87107A
290	D323	Vapor Pressure (lb Reid)	.		
		FLUIDITY			Laboratory Det 13 SA-ALC/SFQLA WPAFB OH 45433
300	D2386	Freezing Point (F)	-		
310	D455	Viscosity at -30 F (cSt) See Below	.		
		COMBUSTION			
400	D1405	Aniline-Gravity Product			GRADE RJ-5
410	D1405	Net Heat of Combustion (Btu/lb)	1 7 8 0 5		
420	D1740	Luminometer Number			REMARKS
430	D1322	Smoke Point	.		
440	D1840	Naphthalenes (vol %)	.		Sample Nbr. 78-17 is satisfactory for Air Force use.
450	D1655	Smoke-Volatility Index	.		
		CORROSION			
500	D130	Copper Strip (2 h at 212F)	1 A		
510	IP227	Silver Strip			Viscosity - CS
		STABILITY			@ 100°F - 13.64
600	D1660	Coker Δ P (in. Hg)	.		@ -30°F - 906.9
610	D1660	Coker Tube Color Code			@ -65°F - 10,000
		CONTAMINANTS			
700	IP225	Copper Content (ug/kg)			Pour Point B - 75°F
710	D381	Existent Gum (mg/100 ml)	9 . 6		
720	D2276	Particulates (mg/liter)	0 . 2		
730	D1094	Water Reaction Vol Change (ml)	.		
740	D1094	Water Reaction Ratings			Supplier: Ashland Chemical
750	D2550	WSIM			
		ADDITIVES	**BRAND**		
800		Anti-icing (vol %)	.		2 x 1 Gal Cans
810		Antioxidant (lb/M bbl)	.		
820		Corrosion Inhibitor (lb/M bbl)	.		
830		Metal Deactivator (lb/M bbl)	.		
840		Antistatic, ppm	.		
		OTHER TESTS			
900	D2624	Conductivity (CU)			APPROVED BY
		Iron, ppm	0		THOMAS J. ... Chief, Aerospace Fuel ... Directorate of Energy Management
		H-nd or RJ-5 Wt. %	9 8 . 8		

AFTO FORM 475   TURBINE FUEL TEST REPORT

Lot #   8285-RJ5G
Gallonage
Date   11-2-78   (by phone)

PROPERTY	RJ-5G TYPICAL PROPERTIES		LOT ANALYSIS
	Min.	MAX.	
Chemical Analysis, Components	H-Norbornadiene Dimers		
Distillation Temperature, °F (°C)			
Initial Boiling Point	–	–	480
5% Point	470 (243)	–	5.12
10% Point	–	–	5.13
20% Point	–	–	5.15
50% Point	–	–	
90% Point	–	–	5.18
End Point, °F (°C)	–	560 (293)	550
Distillation Residue, vol. %	–	1.5	1.0
Distillation Loss, vol. %	–	1.5	1.0
Aromatics, vol. %	–	1.0	
Olefins, vol. %	–	1.0	
Specific Gravity, API (60°/60°)	(1.06)	–	1.089
Existent Gum, mg./100 ml.	–	7.0	9.6
Potential Residue,16 hrs. aging, mg./100 ml.	–	28	
Sulphur, Total, wt. %	–	0.06	0.2
Mercaptan Sulphur, wt. %	–	0.001	
Pour Point, °F	–	~20	-75
Heating Value			17,805
Net Heat of Combustion, BTU/lb.	17,750	–	
Net Heat of Combustion, BTU/gal.	160,000	–	
Iron Content, ppm	–	10	–
Thermal Stability			
Pressure Drop, mm Hg	–	10	
Heater Tube Rating, Visual	–	Code 2	
Viscosity, centistokes			
@ -65°F	–	20,000	10,000
@ -30°F	–	1,400	906.9
@ 100°F	–	15	13.64
Copper Strip Corrosion, ASTM	–	No. 1	1A
Particulate Matter			
mg/liter, F.O.B. origin deliveries	–	1.0	
mg/liter, F.O.B. destination deliveries	–	1.0	.02
Bromine Number	–	–	
Flash Point, °F	150	–	224°F
Water Separometer Index	–	–	

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METHOD	APPEARANCE		RESULTS					SPEC LIMIT	REPORT DATE
10 D156	Color (Saybolt)								**Completed** 5 Nov 79
20	Visual (H-Bright and C-Clear)								CONTRACT NO.
	COMPOSITION								
100 D974	Acidity, Total (mg KOH/g)		•						~~00000000~~ a 79-F-2223
110 D1319	Aromatics (vol %)				•				
120 D1319	Olefins (vol %)			•					DATE SAMPLED 1 Nov 79
130 D1219	Sulfur, Mercaptan (wt %)		•						received 1 Nov 79
140 D484	Doctor Test (p-pos, n-negative)								SAMPLE NO. 9305
150 D1266	Sulfur, Total (wt %)		•						
	VOLATILITY								BATCH NO.
200 D86	Distillation Initial BP (F) **Chemical**								[illegible handwriting]
205	10% Rec (F) **Analysis**								TANK NO.
210	20% Rec (F) JP-10 wt %	4	1	.	0				
215	50% Rec (F) RJ-5 wt %	5	8	.	2				QUANTITY U.S. GALLONS
220	90% Rec (F)								
225	95% Rec (F)								SAMPLING LOCATION
230	Final BP (F)								James R. McCoy
235	Residue (%)		•						Fuels Branch
240	Loss (%)		•						AFAPL/SFF
245	Recovery at 400 F (%)			•					PRODUCT NAME
250 FTMS1151	Explosiveness (vol %)								
260 D56	Flash Point (F) (PM)	1	4	2	Setaflash 144				COMPLIES WITH SPECIFICATION
270 D287	Gravity, API (60 F)		8	.	2				
280 D1289	Gravity, Specific (60/60 F)	1	.	0	1	2	9		**Draft**
290 D323	Vapor Pressure (lb Reid)			•					
	FLUIDITY								DESTINATION
300 D2386	Freezing Pnt (F)			−	6	5		**	
310 D445	Viscosity at -30 F (cSt) -65°F	3	6	6	.	8			**Laboratory**
	COMBUSTION								
400 D1405	Aniline-Gravity Product								GRADE
410 D1405	Net Heat of Combustion (Btu/lb)	1	8	0	2	8			(RJ-6)
420 D1740	Luminometer Number								REMARKS
430 D1322	Smoke Point			•					
440 D1840	Naphthalenes (vol %)		•						Fuel tested as per
450 D1655	Smoke-Volatility Index			•					request.
	CORROSION								
500 D130	Copper Strip (2 h at 212F)								
510 IP227	Silver Strip								
	STABILITY								** Measured by Prof.
600 D1660	Coker Δ P (in. Hg)			•					Moynihan, Catholic U.
610 D1660	Coker Tube Color Code								of America under
	CONTAMINANTS								AFWAL/POSF contract.
700 IP225	Copper Content (ug/kg)								
710 D381	Existent Gum (mg/100 ml)	5	.	•	8				
720 D2276	Particulates (mg/liter)			•					
730 D1094	Water Reaction Vol Change (ml)			•					
740 D1094	Water Reaction Rating								
750 D2550	WSIM								
	ADDITIVES	**BRAND**							
800	Anti-icing (vol %)		•	0	9				
810	Antioxidant (lb/M Bbl)			•					
820	Corrosion Inhibitor (lb/M Bbl)			•					
830	Metal Deactivator (lb/M Bbl)		•						
840	Antistatic, ppm		•						
	OTHER TESTS								
900 D2624	Conductivity (C)								

AFTO FORM 470   TURBINE FUEL TEST REPORT

APPROVED BY
THOMAS J. O'SHAUGHNESSY
Chief, Aerospace Fuels Laboratory
Directorate of Energy Management

RJ-6 TYNDALL

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TABLE A-7. PHYSICAL PROPERTIES OF JP-9

		APPEARANCE	RESULTS	SPEC LIMIT	
					REPORT DATE Completed 12 Apr 78
10	D156	Color (Saybolt)	3 0		CONTRACT NO.
20		Visual (Bright and Clear)			
		COMPOSITION			ORDER NO. 78-F-741
100	D974	Acidity Total (mg KOH/g)			
110	D1319	Aromatics (vol %)			DATE SAMPLED 5 Apr 78
120	D1319	Olefins (vol %)			Rec'd 6 Apr 78
130	D1219	Sulfur, Mercaptan (wt %)			SAMPLE NO.
140	D484	Doctor Test (p, pass, x negative)			3095-5
150	D1266	Sulfur Total (wt %)			BATCH NO.
		VOLATILITY			
200	D86	Distillation Initial BP (F)			TANK NO. Drum D-3-2
205		10% Rec (F)			QUANTITY U.S. GALLONS
210		20% Rec (F)			25 gal to UD
215		50% Rec (F)			SAMPLING LOCATION
220		90% Rec (F)			James McCoy
225		95% Rec (F)			Fuels Branch
230		Final BP (F)			AFAPL/SFF
235		Residue (%)			PRODUCT NAME
240		Loss (%)			Propellant Fuel
245		Recovery at 400 F (Y)			SPECIFICATION
250	D2551	Explosiveness (vol %)			
260	D56	Fl. S Point (F)	6 0		MIL-P-87107A
270	D287	Gravity, API (60 F)	1 7 . 8		
280	D287	Gravity, Specific (60/60 F)			
290	D323	Vapor Pressure (lb Reid)			DESTINATION Laboratory
		FLUIDITY			Det 13 SA-ALC/SFQLA
300	D2386	Freezing Point (F)	B - 6 5		WPAFB OH 45433
310	D445	Viscosity at 30 F (cSt)			
		COMBUSTION			GRADE (JP-9)
400	D1405	Aniline-Gravity Product			REMARKS No Remarks.
410	D1405	Net Heat of Combustion (Btu/lb)	1 8 1 5 1		
420	D1740	Luminometer Number			MCH Wt % - 11.0
430	D1322	Smoke Point			JP-10 Wt % - 67.6
440	D1840	Naphthalenes (vol %)			Hnd Wt % - 20.5
450	D1655	Smoke-Volatility Index			
		CORROSION			
500	D130	Copper Strip (2 h at 212 F)			
510	D1257	Silver Strip			
		STABILITY			
600	D3241	ΔP (mm Hg)	0 . 0		Viscosity CS
610		Coker Tube Color Code	1		0°F -- 9.03
		CONTAMINANTS			-25°F - 14.66
700	D1225	Copper Content (ug/kg)			-65°F - 40.99
710	D381	Existent Gum (mg 100 ml)			
720	D2276	Particulates (mg Gal)	1 . 2		
730	D1094	Water Reaction Vol Change (ml)			Supplier: Suntech Inc
740	D1094	Water Reaction Ratings			
750	D3240	WSIM			1 Gal Jug
		ADDITIVES	BRAND			
800		Anti-icing (vol %)		. 1 3		
810		Antioxidant (lb M Bbl)			
820		Corrosion Inhibitor (lb M Bbl)			
830		Metal Deactivator (lb M Bbl)			
840		Antistatic PPM			
		OTHER TESTS			
900	D2624	Conductivity (cU)		0	
		Iron, PPM			

ITEM	METHOD	APPEARANCE		RESULTS					SPEC LIMIT	
10	D156	Color (Saybolt)	+	2	0					
20		sual (H-Bright and C-Clear)								
		COMPOSITION								
100	D974	Acidity, Total (mg KOH/g)	•							
110	D1319	Aromatics (vol %)				•				
120	D1319	Olefins (vol %)		•						
130	D1219	Sulfur, Mercaptan (wt %)	•							
140	D484	Doctor Test (p'pos, n-negative)								
150	D1266	Sulfur, Total (wt %)	•							
		VOLATILITY								
200	D86	Distillation Initial BP (F) CHEMICAL ANALYSIS								
205		10% Rec (F) JP-10 wt %	9	0	.6					
210		20% Rec (F)								
215		50% Rec (F)								
220		90% Rec (F)								
225		95% Rec (F)								
230		Final BP (F)								
235		Residue (%)		•						
240		Loss (%)		•						
245		Recovery at 400 F (%)			•					
250	FTMS1151	Explosiveness (vol %)								
260	D56	Flash Point (F) P.M.	1	2	6 SETAFLAGH 124°F					
270	D287	Gravity, API (60 F)	1	9	.2					
280	D1289	Gravity, Specific (60/60 F)	0	.	9	3	0	0		
290	D323	Vapor Pressure (lb Reid)		•						
		FLUIDITY								
300	D2386	Freezing Point (F)		-						
310	D455	Viscosity at -30 F (cSt)		•						
		COMBUSTION								
400	D1405	Aniline-Gravity Product								
410	D1405	Net Heat of Combustion (Btu/lb)	1	8	8 7 6					
420	D1740	Luminometer Number								
430	D1322	Smoke Point			•					
440	D1840	Napthalenes (vol %)		•						
450	D1655	Smoke-Volatility Index			•					
		CORROSION								
500	D130	Copper Strip (2 h at 212F)								
510	1P227	Silver Strip								
	D-3241	**STABILITY**								
600	JFTOT	Coker Δ P (in. Hg)		0	.0					
610	JFTOT	Coker Tube Color Code	4	1	T.D.R.= 4.0					
		CONTAMINANTS								
700	1P225	Copper Content (ug/kg)								
710	D381	Existent Gum (mg/100 ml)	1	.0						
720	D2276	Particulates (mg/liter)	1	.5						
730	D1094	Water Reaction Vol Change (ml)			•					
740	D1094	Water Reaction Ratings								
750	D2550	WSIM								
		ADDITIVES	**BRAND**							
800	Anti-icing (vol %)		+	1	8					
810	Antioxidant (lb/M Bbl)			•						
820	Corrosion Inhibitor (lb/M Bbl)			•						
830	Metal Deactivator (lb/M Bbl)			•						
840	Antistatic, ppm			•						
		OTHER TESTS								
900	D2624	Conductivity (CU)								

REPORT DATE COMPLETED
6 Nov 1979

CONTRACT NO.
73-D-0023

ORDER NO.
79-F-2233

DATE SAMPLED 1 Nov 79

RECD 2 Nov 79

SAMPLE NO.
79-28

BATCH NO.
9304

TANK NO.
8

QUANTITY U.S. GALLONS
1568

SAMPLING LOCATION
QAS OPNS Branch Cols
c/o DCSC Bldg 1, Sec 1
Columbus OH 43215

PRODUCT NAME
Propellant Fuel

COMPLIES WITH SPECIFICATION

MIL-P-87107A

ORGANIZATION LABORATORY
Det 1 3 SA-ALC/SFQLA
Aerospace Fuels Lab
WPAFB OH 45433

GRADE
JP-10

REMARKS

Fuel Does not meet
specification
requirements for total
solids. *Solids removed before shipment*

VISCOSITY cs
@ 0°F   3.26
@-65°F   35.09

SUPPLIER:
Ashland Chemical
2X1 Gal Can

APPROVED BY
THOMAS J. O'SHAUGHNESSY
Chief, Aerospace Fuels Laboratory
Directorate of Energy Management

AFTO FORM 476   TURBINE FUEL TEST REPORT

Appendix B

EXPERIMENTAL METHODS

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DETAILS OF ANALYTICAL METHODS

Fuel Analysis by Capillary Column Gas Chromatography

The split injection analyses were performed on a Hewlett Packard Model 5840A gas chromatograph, FID detector under the following conditions:

Column: 30-m x 0.25-mm-ID SE-30 (WCOT methyl silicone gum)

Carrier gas: He at 1.5 ml min^{-1}

Split ratio: 200:1 (300 ml min^{-1} He ejected through injector vent)

Column temperature program: Initial T: 10°C for 5 min

Program rate: 5°C min^{-1}

Final T: 210°C

Injector temperature: 250°C

Detector temperature: 250°C

Injection of neat samples (0.1 μl) of JP-4, JP-5, and JP-8 was made for the quantitative determinaton of fuel composition.

The splitless injection analyses were also conducted on a Hewlett Packard Model 5840A gas chromatograph, FID detector under the following conditions:

Column: 30-m x 0.25-mm-ID SE-30 (WCOT methyl silicone gum)

Carrier gas: He at 0.75 ml min^{-1}

Column temperature program: Initial T: 30°C for 10 min

Program rate: 4.5° min^{-1}

Final T: 210°C

The detailed steps of the analysis are given below:

1. Injection of the pure fuels in CS_2 solutions for JP-4, JP-5, JP-8, RJ-4, RJ-5, RJ-6, JP-9 and JP-10. Sample preparation: For JP-4, JP-5, and JP-8, solutions were prepared containing 0.4 μl ml^{-1} of fuel in CS_2 with 9.5 μg ml^{-1} n-octadecane added as an internal standard. For RJ-4, RJ-5, RJ-6, JP-9 and JP-10, solutions of 0.1 μl ml^{-1} of fuel in CS_2 were prepared, again

with 9.5 $\mu g\ ml^{-1}$ n-octadecane added as an internal standard. Injected sample size in each case was 1 μl.

2. Injection of the pure fuels in CS_2 solutions, with normal alkanes n-heptane to n-octadecane added for Kovats indices assignments. Sample preparation: CS_2 solutions of the fuels were prepared as in Step 1 with the addition of approximately 10 $\mu l\ ml^{-1}$ per component of normal alkanes from n-heptane to n-octadecane. Injected sample size was 1 μl.

3. Quantitation of the major water-soluble fuel components par-titioned into deionized water and artificial seawater from a 1:1000 fuel:water equilibration at 20°C. Sample prepara-tion: 100 ml of water were added to a 150-ml capacity Corex® centrifuge tube. 100 μl of fuel were injected from a syringe into the water to disperse the fuel as tiny droplets in the water phase. The centrifuge tube was sealed with a screw cap containing a Teflon liner, then attached to a propeller-type stirrer. The propeller shaft with attached sample tubes was submerged in a constant temperature bath set at 20°C and the samples were rotated gently for 48 hours. Following equilibration, the tubes were centrifuged for 30 minutes at 5000 rpm, which produced a relative centrifugal force of approximately 1500 g at the solution surface and 3500 g at the bottom of the tube. The bulk fuel was siphoned from the surface of the water to prevent fuel contamination on the sampling pipet, and a 5-ml sample was immediately transferred to a 15-ml capacity conical centrifuge tube. 250 μl of CS_2 contain-ing 9.5 $\mu g\ ml^{-1}$ n-octadecane were immediately injected into the water sample, and the mixture was spun on a vortex mixer for 30 seconds to ensure complete extraction. This mixture was centrifuged for 30 seconds in a clinical centrifuge and the CS_2 extract coalesced at the bottom of the tube. The extracted sample was kept beneath the aqueous phase to prevent CS_2 evapora-tion.

4. Quantitation of the major water-soluble fuel components of JP-4, JP-8, and JP-9 partitioned from a 1:1000 fuel:water equilibration at 4°C and 30°C. Samples were prepared as described in Step 3 with both deionized water and artificial seawater.

5. Quantitation of the major water-soluble fuel components of JP-4, JP-8, and JP-9 partitioned from a 20°C equilibration at 1:10, 1:100, and 1:10,000 fuel:water mixtures. 100 ml of deionized water and artificial seawater were used in preparation of the 1:10 and 1:100 fuel:water mixtures, and 150 ml of water were used for the 1:10,000 mixture. Otherwise, sample preparation was as described in Step 3.

6. Volatilization of the water-soluble fuel components of JP-4, JP-8, and JP-9 partitioned from a 1:1000 fuel:water equilibration at 20°C. Following equilibration, 75 ml of solution from each of 6 tubes were transferred by pipet to a 600-ml beaker with a minimum of turbulence. A calibrated oxygen probe was inserted just below the surface of the water so as not to disturb the vortex during volatilization. A constant speed, propeller-type stirrer was used for solution stirring. During volatilization, 5-ml samples were removed at appropriate time intervals and transferred to 15-ml capacity conical centrifuge tubes. These samples were immediately extracted with CS_2 as described in Step 3. When slower stirring speeds were used, samples were collected at 0, 10, 20, 30, 40, 60, and 80 min. With faster stirring speeds, collection times were 0, 6, 12, 18, 24 and 30 min. Following collection of the last sample, N_2 was introduced to the solution through a fritted glass dispersion tube, which purged the oxygen from the solution. Without changing the stirring rate, the rate of change of the oxygen concentration was monitored with a dissolved oxygen analyzer.

7. Photolysis of the water-soluble components of JP-4 parti-
tioned from a 1:1000 fuel:water equilibration at 20°C.
Aqueous solutions of JP-4 were prepared as described in
Step 3 in each of three waters: deionized water, fresh
pond water from Searsville Pond in Portola Valley, CA,
and seawater from Santa Cruz, CA. Before being mixed through
a medium porosity glass filer, the sample is centrifuged
at 5000 rpm (relative centrifugal force range in tube of
1500 g to 3500 g) for 30 minutes and finally refiltered
through a 0.20-μm membrane filter. This ensured the
removal of suspended particles and microbes. Following
equilibration with the bulk fuel, the water solutions were
transferred by pipet to quartz tubes, which were filled to
the brim and sealed with screw-caps containing Teflon®-lined
septa. Care was taken to avoid a head space or the trap-
ping of air bubbles, which could allow fuel components to
volatilize during the experiment.

The tubes were placed on a rack inclined 30° from
the horizontal toward the south. A second identical
series of tubes was prepared with each tube wrapped with
aluminum foil to exclude light. Sets of six photolysis
tubes were analyzed after 7, 14, and 21 days of light
exposure. Each set consisted of one exposed and one
dark control for each water. A 5-ml sample was removed
from each tube and immediately extracted with CS_2 as
described in Step 3. As with the other studies, the CS_2
contained n-octadecane as an internal standard.

GC-MS Analysis

Jet fuel samples were analyzed on a Finnigan 3200 gas chromatograph/
mass spectrometer with an electron impact ion source and with an Alpha-16
model 6100 data system. The column used was a 37-m x 0.21-mm-ID SP-2100
fused silica capillary column.

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(Hewlett Packard). The column was put through the GC/MS interface directly to the ion source. Helium was used as the carrier gas at a column head pressure of 13 psig.

A Grob-type capillary column inlet was used. When used in the splitless mode, a 2-μl aliquot of the sample was injected with the shut-off valve closed. At 30 seconds the shut-off valve was opened, allowing the continuous venting of the injector system by 30 cm^3 min^{-1} of carrier gas. When split injection samples were run, the carrier gas flow rate through the splitter valve was set at 200 cm^3 min^{-1} and 0.1 μl of neat sample was injected.

Ionization was conducted at 68-74 ev with an emission current of 0.55 mA. The scan rate was set at maximum speed, about one scan per second. The exact scan rate was calculated for each run.

The temperature program and the data acquisition times for the various runs were varied according to the anticipated type of sample.

Each day, a quality control run of 20 ng of decafluorotriphenyl-phosphene was run.[1] Its ion fragments were checked and compared with recent runs to ensure adequate sensitivity.

Separation of Aliphatic and Aromatic Components of Jet Fuels[2]

The aliphatic and aromatic hydrocarbons of JP-4, JP-5, and JP-8 were separated by silica gel column chromatography. The silica gel (Accurate Chemical and Scientific Corp., 90-200 mesh) was activated at 155°C for five days. (This step is probably not necessary.) Hydrocarbon traces were removed by boiling the activated silica gel in several volumes of methylene chloride for 10 minutes and filtering the slurry in a Buchner funnel. The silica gel was then dried and activated at 155°C for an additional three days. Distilled-in-glass quality solvents (Burdick and Jackson Laboratories, Inc.) were used without purification throughout the work.

[1] W. Budde and J. Eichelberger, "An EPA Manual for Organic Analysis Using Gas Chromatography Mass Spectrometry" EPA Report No. 600/8-79-006 (March 1979), p. 16, 17.

[2] J. S. Warner, Anal. Chem., 48 (3), 579 (1976).

A glass chromatography column (0.9 cm ID) with a Teflon® stopcock
was plugged with methylene cloride-washed glass wool. The washed and
activated silica gel (10.0 g) was added to 50 ml n-hexane for one hour
with periodic stirring to remove bubbles. The silica gel-hexane slurry
was added to the column and allowed to settle. The stopcock was opened
until the solvent level was about 1 mm above the silica gel. A 100-μl
aliquot of the jet fuel was deposited on the top of the silica gel column
with minimum disturbance to the surface layer. The solvent level was
again reduced to 1 mm above the silica gel and 25 ml n-hexane were added.
The eluate was collected at a rate of 1 to 2 ml min^{-1} in a 250-ml volu-
metric flask. This first fraction contains the saturated aliphatic
hydrocarbons and probably the olefins.

Then, a 50-ml aliquot of a 20% methylene chloride/80% n-hexane
solution (v/v) was added to the top of the column. Two 25-ml fractions
were collected in 25-ml volumetric flasks. Fraction 2 contains the mon-
and diaromatic hydrocarbons. Fraction 3 will contain most of the triaro-
matic hydrocarbons.

Appendix C

GAS CHROMATOGRAPHY AND GAS CHROMATOGRAPHY-MASS SPECTROMETRY DATA

Fuel Components	Kovats Index
n-Butane	400.0
Isobutane	466.3
n-Pentane	500.0
2,2-Dimethylbutane	527.7
2-Methylpentane	562.4
3-Methylpentane	578.7
n-Hexane	600.0
Methylcyclopentane	622.0
2,2-Dimethylpentane	629.1
Benzene	644.5
Cyclohexane	653.6
2-Methylhexane	669.5
3-Methylhexane	677.3
trans-1,3-Dimethylcyclopentane	679.6
cis-1,3-Dimethylcyclopentane	681.9
cis-1,2-Dimethylcyclopentane	684.4
n-Heptane	700.0
Methylcyclohexane	715.1
2,2,3,3-Tetramethylbutane	720.5
Ethylcyclopentane	729.8
2,5-Dimethylhexane	737.3
2,4-Dimethylhexane	738.4
1,2,4-Trimethylcyclopentane	740.8
3,3-Dimethylhexane	743.3
1,2,3-Trimethylcyclopentane	748.1
Toluene	753.0
2,2-Dimethylhexane	764.2
2-Methylheptane	772.0
4-Methylheptane	772.7
cis-1,3-Dimethylcyclohexane	775.3
3-Methylheptane	778.0
1-Methyl-3-ethylcyclohexane	784.1
1-Methyl-2-ethylcyclohexane	786.7
Dimethylcyclohexane	788.8
n-Octane	800.0
1,3,5-Trimethylcyclohexane	825.3
1,1,3-Trimethylcyclohexane	831.0
2,5-Dimethylheptane	833.6
Ethylbenzene	844.9
m-Xylene	853.9
p-Xylene	854.8
3,4-Dimethylheptane	859.8
4-Ethylheptane	865.0
4-Methyloctane	868.5
2-Methyloctane	869.6
3-Methyloctane	873.9
o-Xylene	875.3
1-Methyl-4-ethylcyclohexane	881.3
n-Nonane	900.0
Isopropylbenzene	905.1
n-Propylbenzene	937.2
1-Methyl-3-ethylbenzene	944.9
1-Methyl-4-ethylbenzene	946.8

Peak time labels visible on chromatogram: 1.39, 1.68, 1.85, 2.17, 2.52, 2.57, 2.65, 2.91, 3.02, 3.29, 3.98, 4.12, 4.64, 4.98, 5.63, 5.98, 6.32, 7.13, 7.66, 7.89, 8.26, 8.62, 9.04, 9.26, 9.59, 9.79, 10.17, 10.27, 10.48, 11.05, 11.39, 11.68, 12.61, 13.18, 13.75, 14.08, 14.42, 14.67, 14.94, 15.64, 15.81, 15.98, 16.57, 16.78, 17.10, 17.38

Figure C-1.   Split Injection GC Analysis of JP-4 with Peak Assignments

Fuel Components	Kovats Index
1,3,5-Trimethylbenzene	952.8
1-Methyl-2-ethylbenzene	961.0
1,2,4-Trimethylbenzene	975.6
n-Decane	1000.0
n-Butylcyclohexane	1025.6
1,3-Diethylbenzene	1031.4
1-Methyl-4-propylbenzene	1034.7
1,3-Dimethyl-5-ethylbenzene	1041.6
1-Methyl-2-i-propylbenzene	1049.1
1,4-Dimethyl-2-ethylbenzene	1060.2
1,2-Dimethyl-4-ethylbenzene	1067.1
n-Undecane	1100.0
1,2,3,4-Tetramethylbenzene	1128.8
Naphthalene	1156.5
2-Methylundecane	1166.0
n-Dodecane	1200.0
2,6-Dimethylundecane	1216.1
2-Methylnaphthalene	1265.7
1-Methylnaphthalene	1276.4
n-Tridecane	1300.0
2,6-Dimethylnaphthalene	1379.4
n-Tetradecane	1400.0
n-Pentadecane	1500.0
n-Hexadecane	1600.0

Peak retention time labels: 17.67, 18.14, 18.45, 19.54, 19.52, 20.02, 20.34, 20.53, 20.64, 20.87, 21.12, 21.50, 21.74, 21.93, 22.92, 23.32, 23.79, 24.46, 24.66, 24.96, 25.15, 26.08, 26.53, 27.87, 28.29, 29.01, 31.20, 31.78, 31.92, 33.47, 33.63, 34.23, 34.37, 36.84

Figure C-1.   Split Injection GC Analysis of JP-4 with Peak Assignments (Concluded)

Fuel Components	Kovats Index	
Isobutane	466.3	1.68
n-Pentane	500.0	1.85
2-Methylpentane	562.4	2.56
3-Methylpentane	578.7	2.91
n-Hexane	600.0	3.29
Methylcyclopentane	622.0	3.98
Cyclohexane	653.6	4.98
2-Methylhexane	669.5	5.63
3-Methylhexane	677.3	5.99
cis-1,2-Dimethylcyclopentane	684.4	6.32
n-Heptane	700.0	7.18
Methylcyclohexane	715.1	7.66
Toluene	753.0	9.25
2-Methylheptane	772.0	10.17
3-Methylheptane	778.0	10.45
Dimethylcyclohexane	788.8	11.04
		11.39
n-Octane	800.0	11.64
1,3,5-Trimethylcyclohexane	826.1	12.68
1,1,3-Trimethylcyclohexane	831.8	12.92
Ethylbenzene	844.9	13.17
		13.45
w-Xylene	854.4	13.73
3-Methyloctane	869.8	13.98
2,4,6-Trimethylheptane	874.4	14.28
o-Xylene	875.5	14.54
		15.02
n-Nonane	900.0	15.63 15.77
		15.97
		16.18
		16.33
		16.88
		17.48
1,2,4-Trimethylbenzene	975.7	18.22 18.52
n-Decane	1000.0	19.58
n-Butylcyclohexane	1025.4	20.01 20.32
1,3-Diethylbenzene	1031.2	
1,3-Dimethyl-5-ethylbenzene	1041.2	20.85
1,4-Dimethyl-2-ethylbenzene	1060.1	
2-Methyldecane	1063.1	21.50
1-Ethylpropylbenzene	1066.5	21.92 21.72

Figure C-2.   Split Injection GC Analysis of JP-5 with Peak Assignments

111

Fuel Components	Kovats Index	
n-Undecane	1100.0	
		22.93
2,6-Dimethyldecane	1113.1	
1,2,3,4-Tetramethylbenzene	1128.3	23.78
Naphthalene	1156.5	
2-Methylundecane	1165.9	24.96
		25.14
n-Dodecane	1200.0	26.08
2,6-Dimethylundecane	1216.0	
1,2,4-Triethylbenzene	1223.4	26.53
2-Methylnaphthalene	1265.2	
1-Methylnaphthalene	1275.8	28.28
1-Tridecene	1289.6	
Phenylcyclohexane	1293.2	29.02
n-Tridecane	1300.0	
1-t-Butyl-3,4,5-trimethylbenzene	1306.8	
n-Heptylcyclohexane	1336.9	
n-Heptylbenzene	1348.6	
Biphenyl	1351.9	
1-Ethylnaphthalene	1368.0	
2,6-Dimethylnaphthalene	1379.4	31.19
n-Tetradecane	1400.0	31.78
2,3-Dimethylnaphthalene	1410.4	
n-Octylbenzene	1450.0	
		33.45
n-Pentadecane	1500.0	34.37
n-Hexadecane	1600.0	36.56 36.81
n-Heptadecane	1700.0	39.14 39.36
n-Octadecane	1800.0	41.35

Figure C-2. Split Injection GC Analysis of JP-5 with Peak Assignments (Concluded)

112

Fuel Component	Kovats Index	
n-Butane	400.0	1.39
Isobutane	466.3	1.57
n-Pentane	500.0	1.85
2-Methylpentane	562.4	2.66
3-Methylpentane	578.7	2.89
n-Hexane	600.0	3.29
Methylcyclopentane	622.0	3.89
2-Methylhexane	669.5	5.61
3-Methylhexane	677.3	5.96
n-Heptane	700.0	7.09
Methylcyclohexane	715.1	7.65
1,2,3-Trimethylcyclopentane	748.1	9.03
Toluene	753.0	9.24
2-Methylheptane	772.0	10.13
3-Methylheptane	778.0	10.43
1-Methyl-2-ethylcyclohexane	786.7	
Dimethylcyclohexane	788.8	10.83
n-Octane	800.0	11.39 / 11.63
		12.58
1,3,5-Trimethylcyclohexane	825.9	12.91
1,1,3-Trimethylcyclohexane	831.9	13.15
m-Xylene	854.5	13.34
		13.72
		13.97
3-Methyloctane	870.0	14.23
2,4,6-Trimethylheptane	874.3	14.60
o-Xylene	875.7	14.91
cis-1-Ethyl-3-methylcyclohexane	881.9	15.21
		15.61 / 15.75
n-Nonane	900.0	15.95
n-Propylcyclohexane	923.0	
		17.30
1,2,4-Trimethylbenzene	975.5	18.50
n-Decane	1000.0	19.49
		20.00
n-Butylcyclohexane	1025.4	20.31
1,3-Dimethyl-5-ethylbenzene	1041.2	20.49 / 20.84
1,4-Dimethyl-2-ethylbenzene	1060.1	
2-Methyldecane	1063.0	21.49
1-Ethylpropylbenzene	1066.4	21.71

Figure C-3. Split Injection GC Analysis of JP-8 with Peak Assignments

113

Fuel Component	Kovats Index
n-Undecane	1100.0
2,6-Dimethyldecane	1119.0
1,2,3,4-Tetramethylbenzene	1128.1
Naphthalene	1155.9
2-Methylundecane	1165.2
n-Dodecane	1200
1,3,5-Triethylbenzene	1203.8
2,6-Dimethylundecane	1215.7
1,2,4-Triethylbenzene	1222.7
n-Hexylcyclohexane	1236.6
2-Methylnaphthalene	1264.8
1-Methylnaphthalene	1275.5
1-Tridecene	1289.3
Phenylcyclohexane	1292.6
n-Tridecane	1300.0
n-Heptylcyclohexane	1336.7
n-Heptylbenzene	1347.7
Biphenyl	1351.3
1-Ethylnaphthalene	1367.2
2,6-Dimethylnaphthalene	1378.9
n-Tetradecane	1400.0
2,3-Dimethylnaphthalene	1410.4
n-Octylbenzene	1450.6
n-Pentadecane	1500.0
n-Hexadecane	1600.0
n-Heptadecane	1700.0
n-Octadecane	1800.0

Figure C-3.   Split Injection GC Analysis of JP-8 with Peak Assignments (Concluded)

114

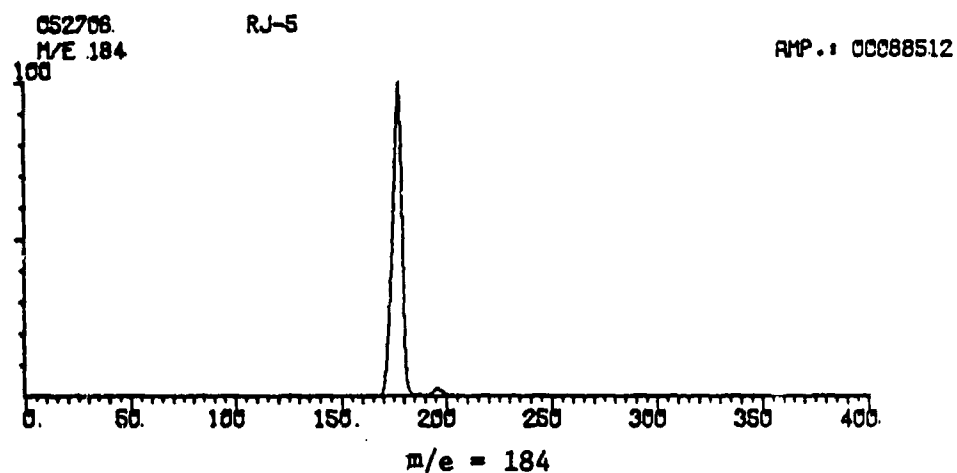Figure C-4. GC-MS Traces of RJ-4 at Three Specific M/E Values

115

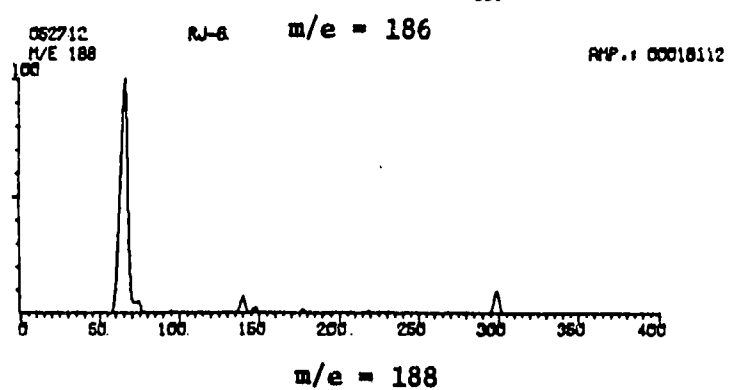Figure C-5. GC-MS Traces of RJ-5 at Three Specific M/E Values

116

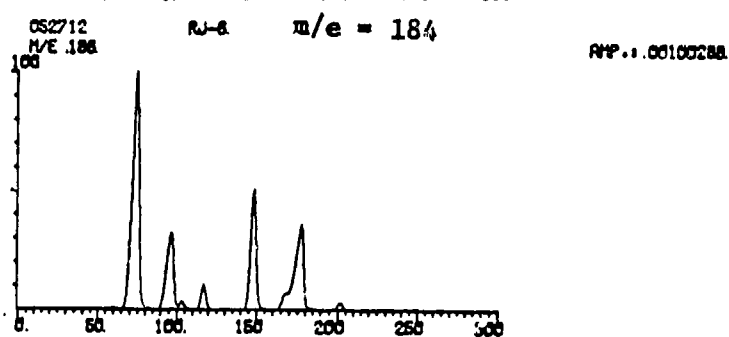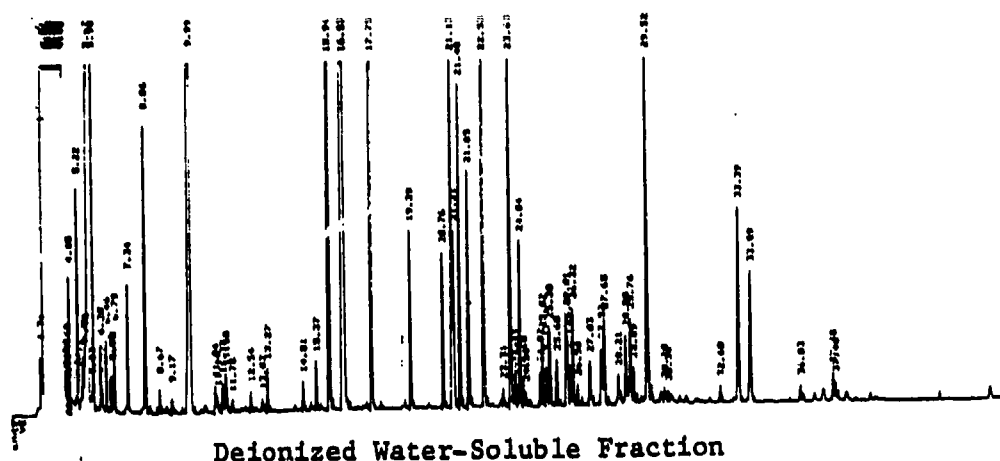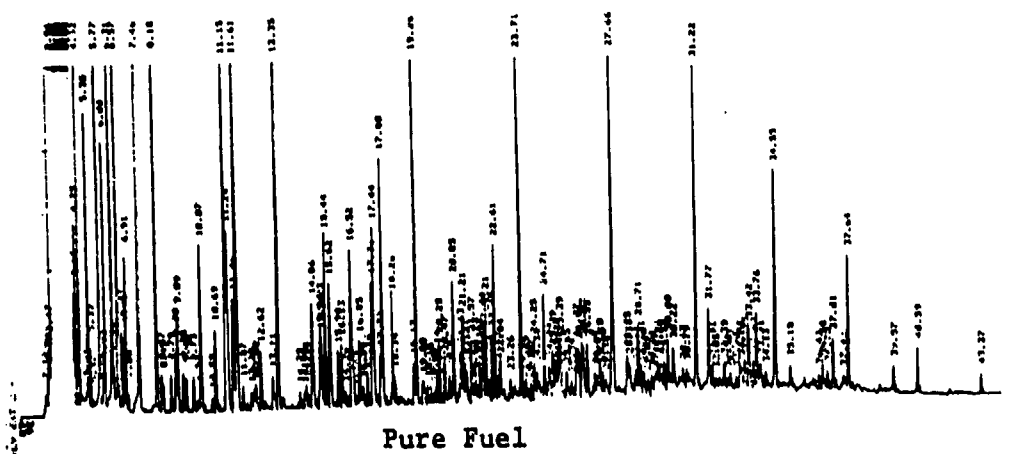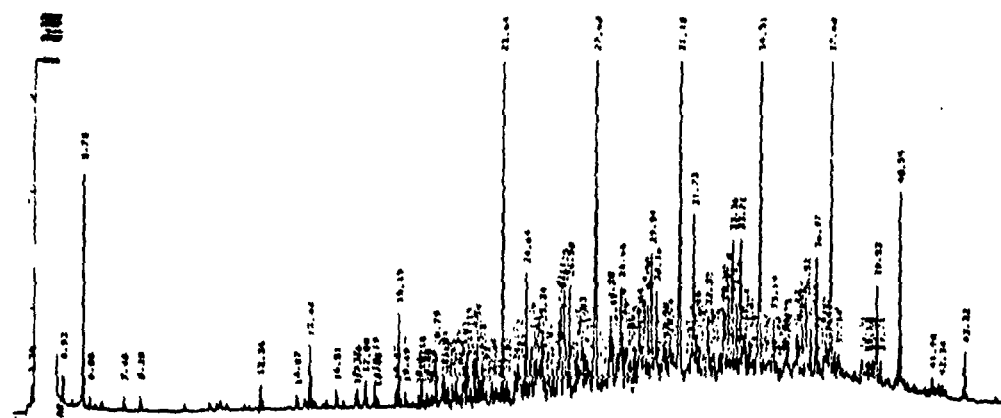Figure C-6. GC-MS Traces of RJ-6 at Four Specific M/E Values

117

Pure Fuel

Deionized Water-Soluble Fraction

Synthetic Seawater-Soluble Fraction

Figure C-7. GC Traces of JP-4 in CS_2

118
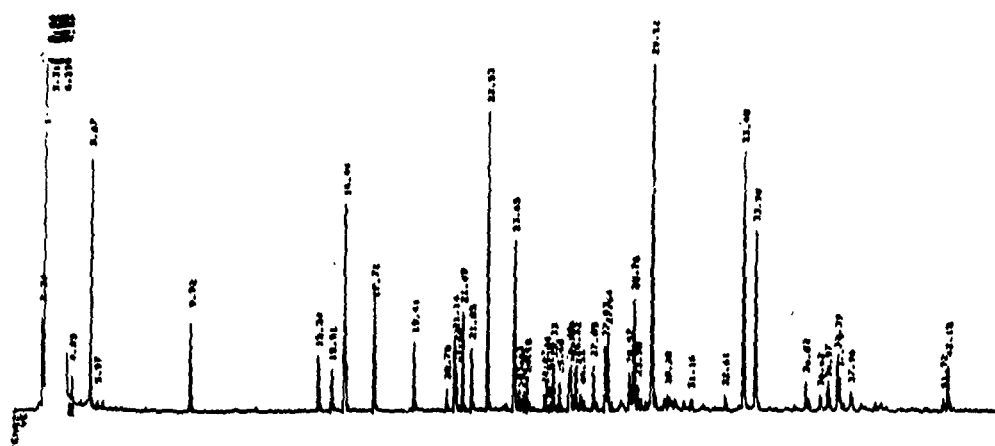
Pure Fuel

Deionized Water-Soluble Fraction

Synthetic Seawater-Soluble Fraction

Figure C-8. GC Traces of JP-5 in CS_2

119

Pure Fuel
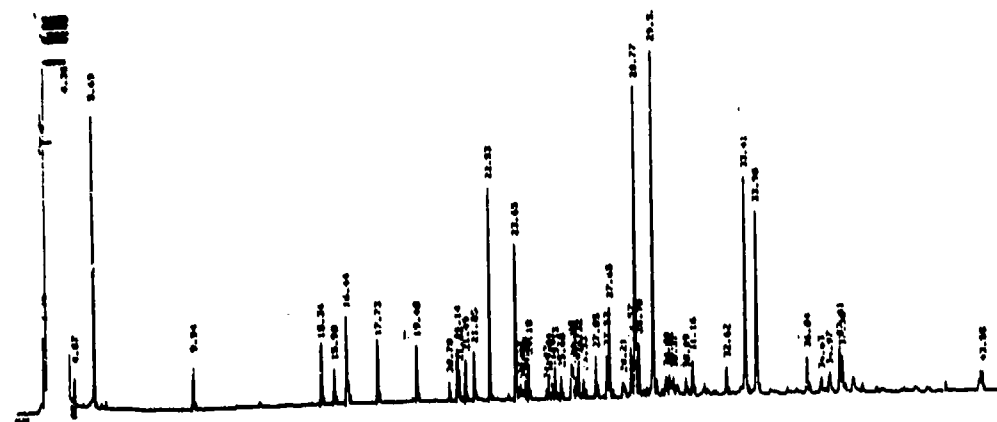
Deionized Water-Soluble Fraction
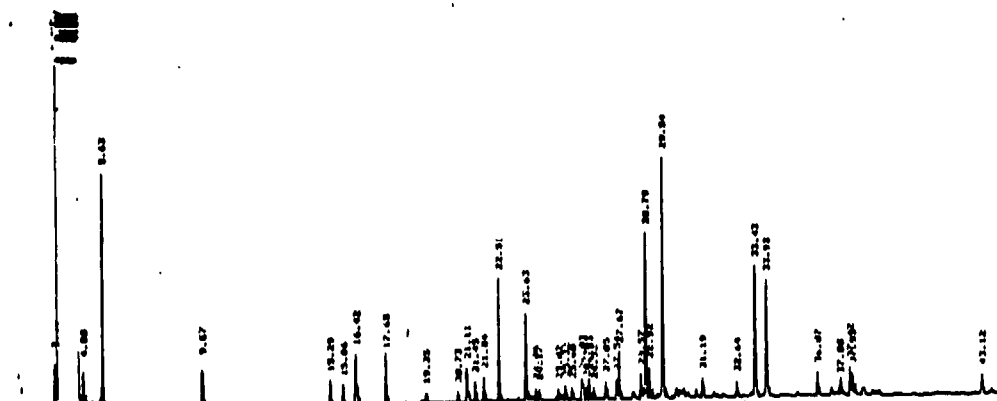
Synthetic Seawater-Soluble Fraction

Figure C-9, GC Traces of JP-8 in CS_2

120

Pure Fuel

Deionized Water-Soluble Fraction

Synthetic Seawater-Soluble Fraction

Figure C-10. GC Traces of RJ-4 in CS_2
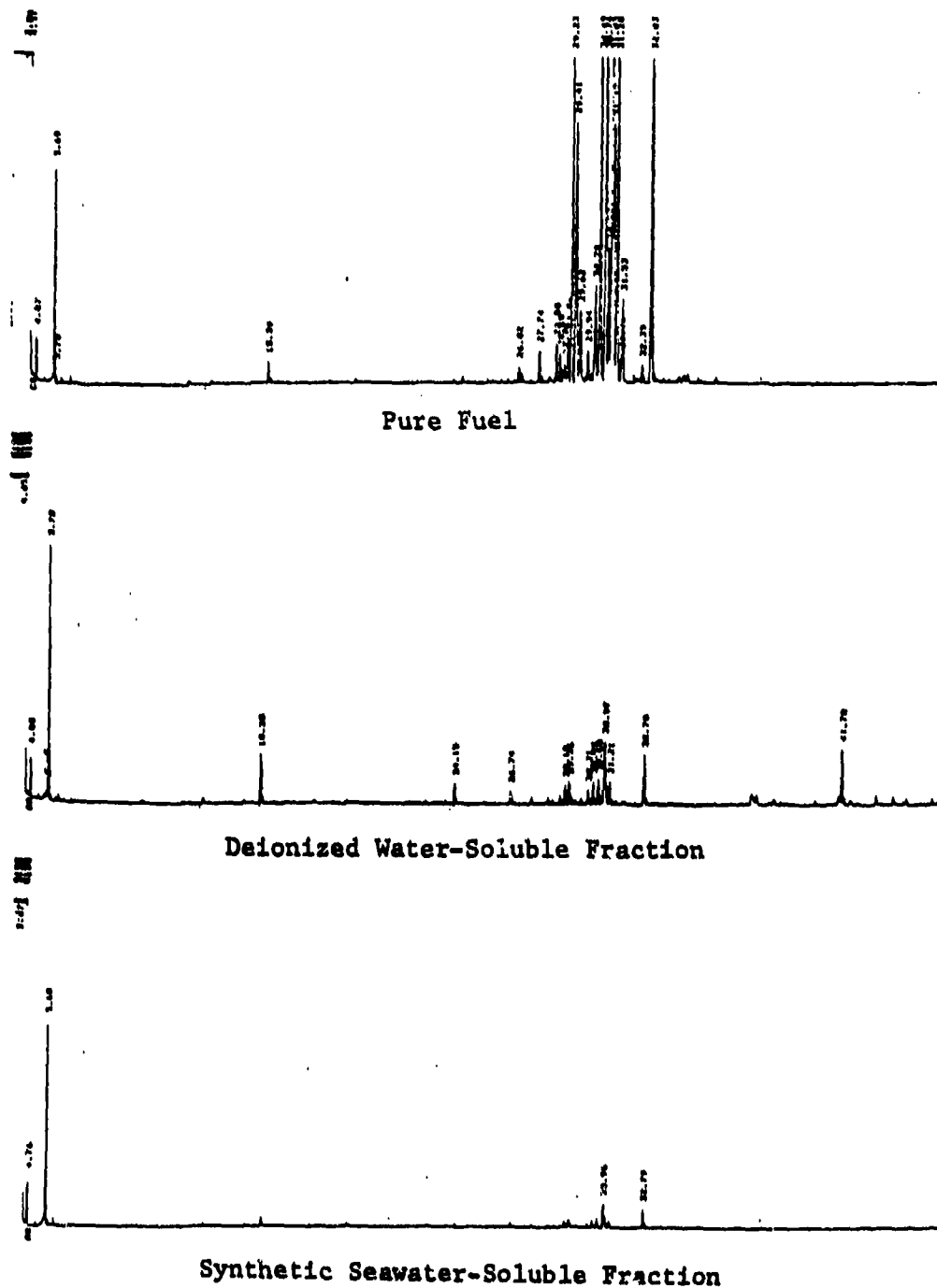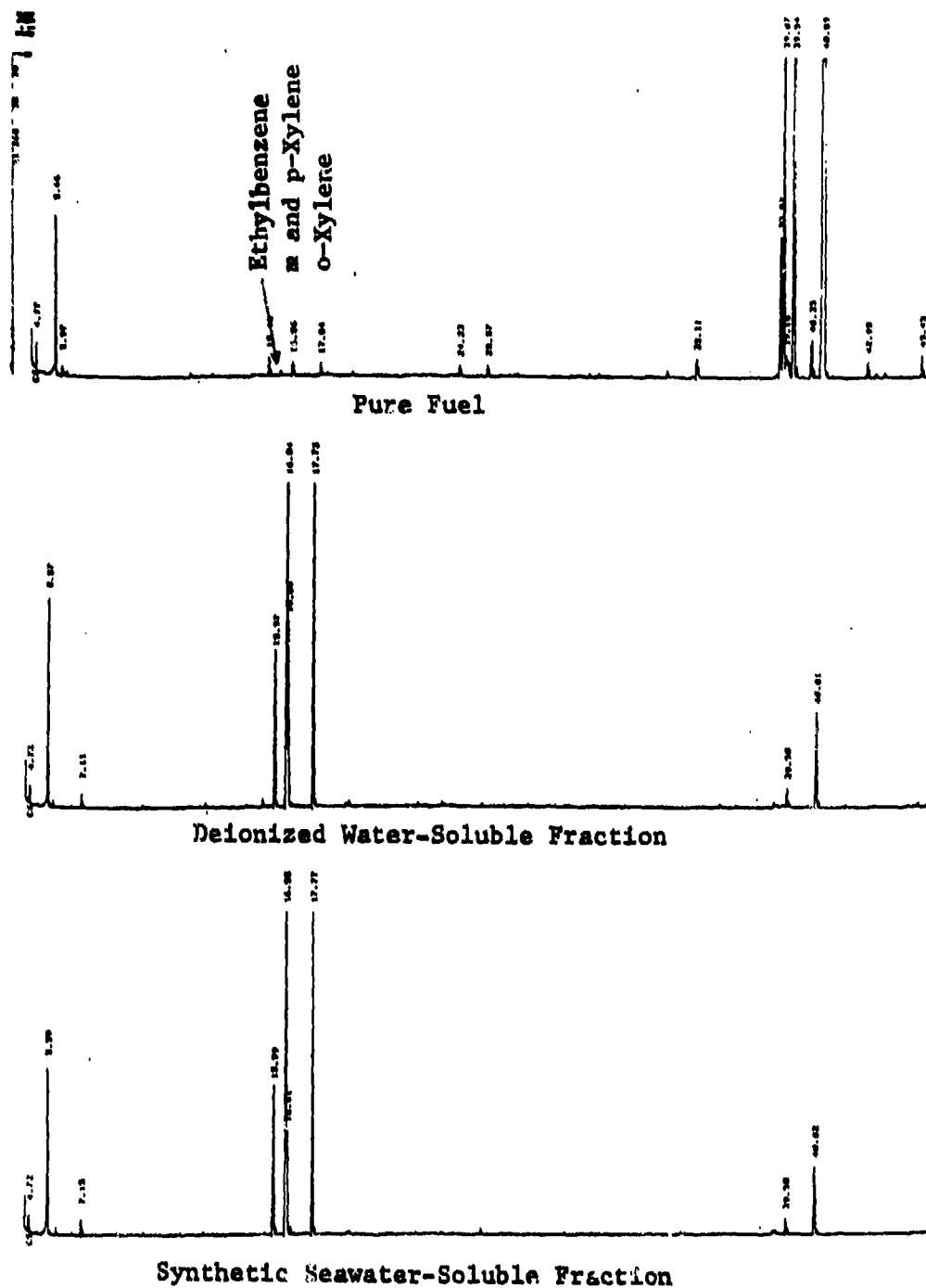
Figure C-11. GC Traces of RJ-5 in CS_2
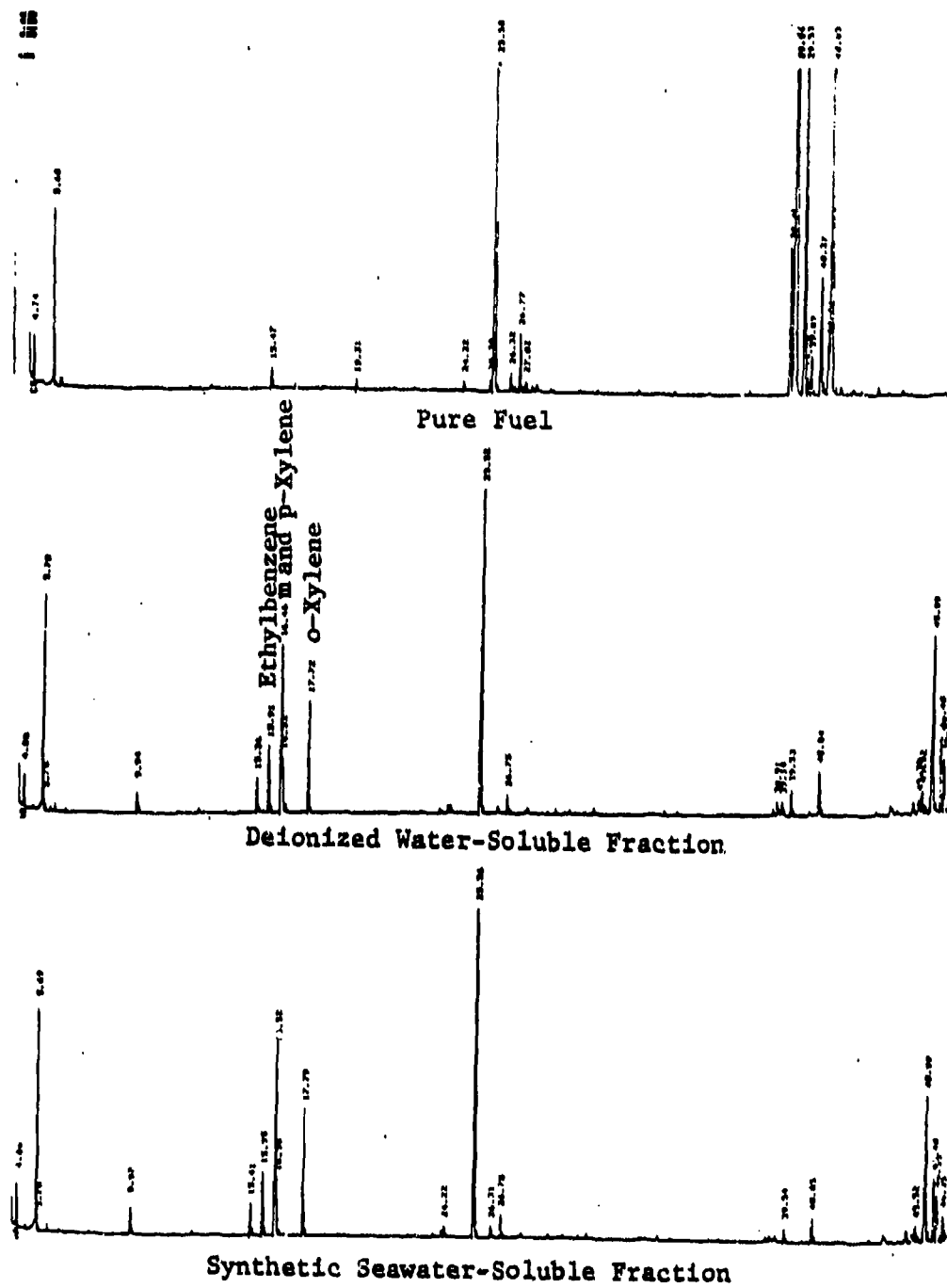
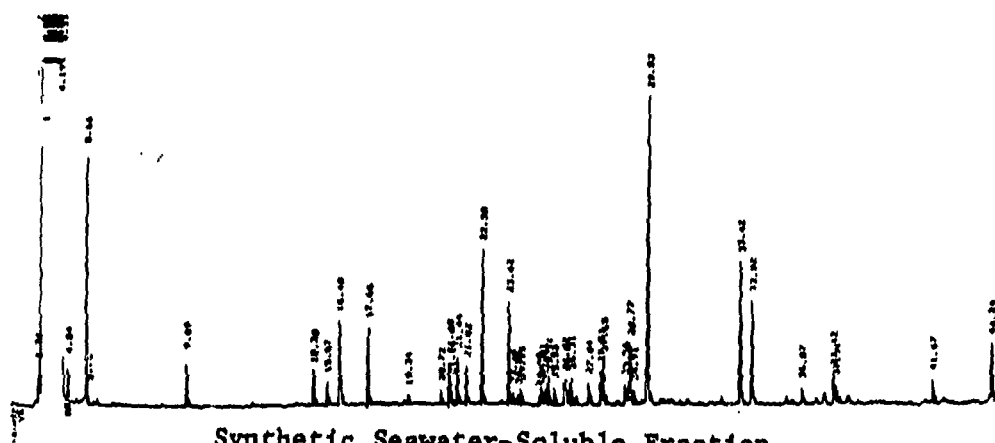Figure C-12. GC Traces of RJ-6 in CS_2

123

Pure Fuel

Deionized Water-Soluble Fraction

Synthetic Seawater-Soluble Fraction

Figure C-13. GC Traces of JP-9 in CS_2

124

Pure Fuel

Ethylbenzene
m and p-Xylene
o-Xylene
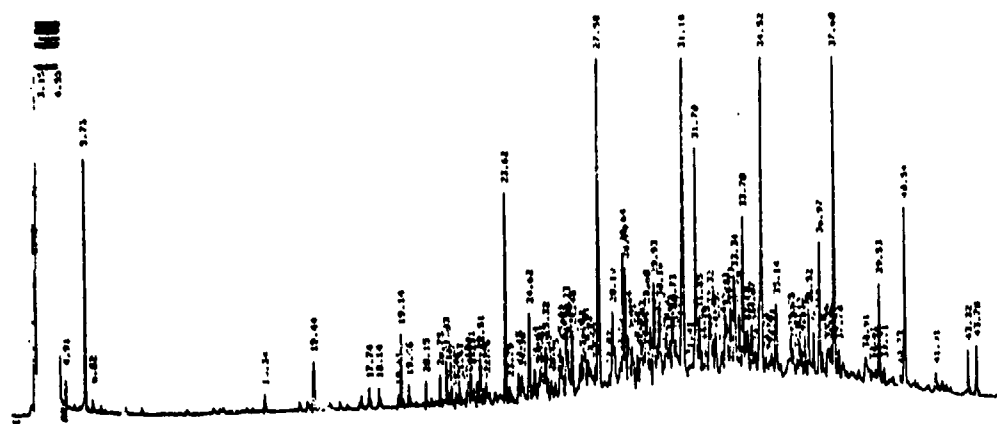
Deionized Water-Soluble Fraction

Synthetic Seawater-Soluble Fraction
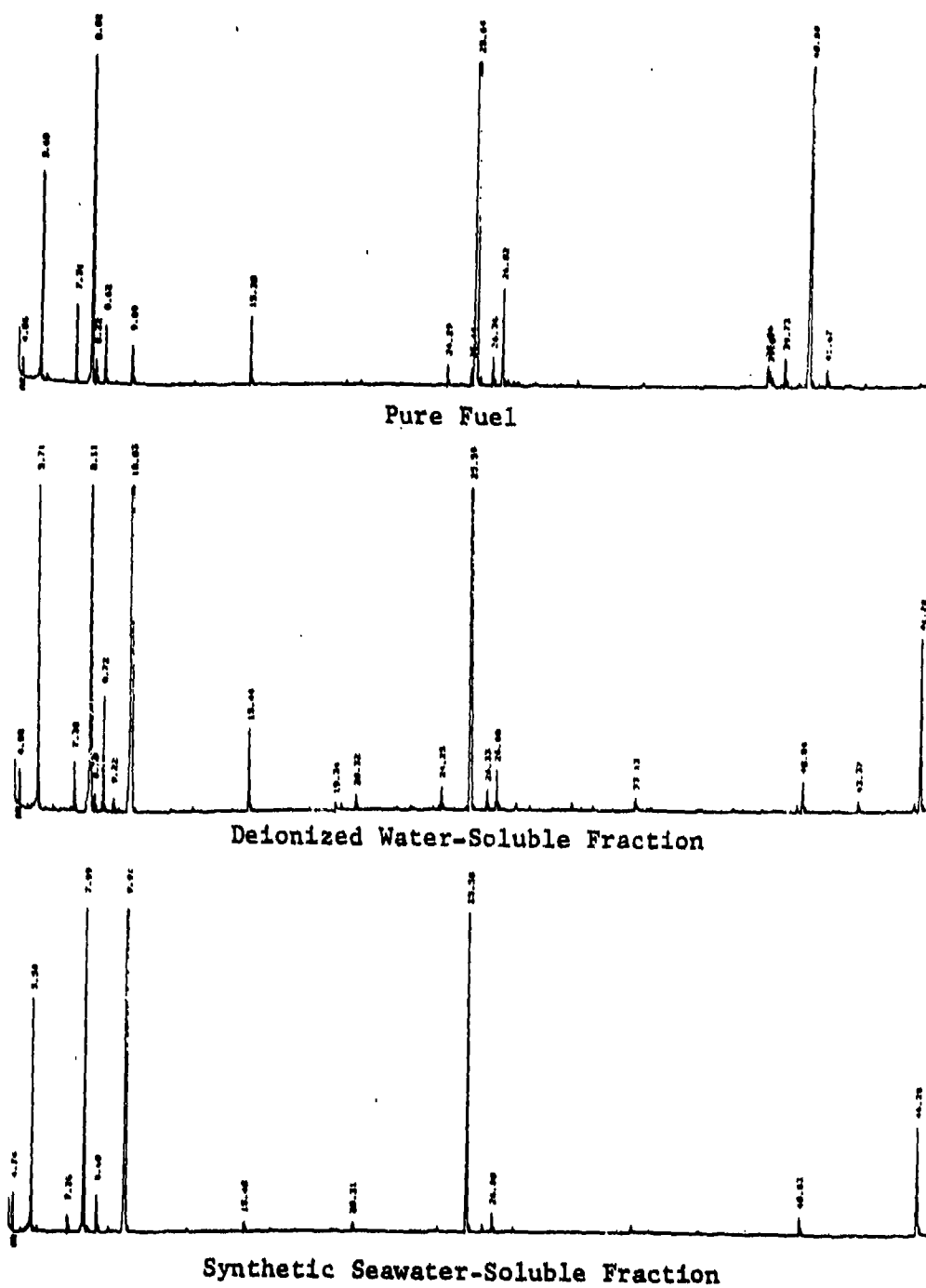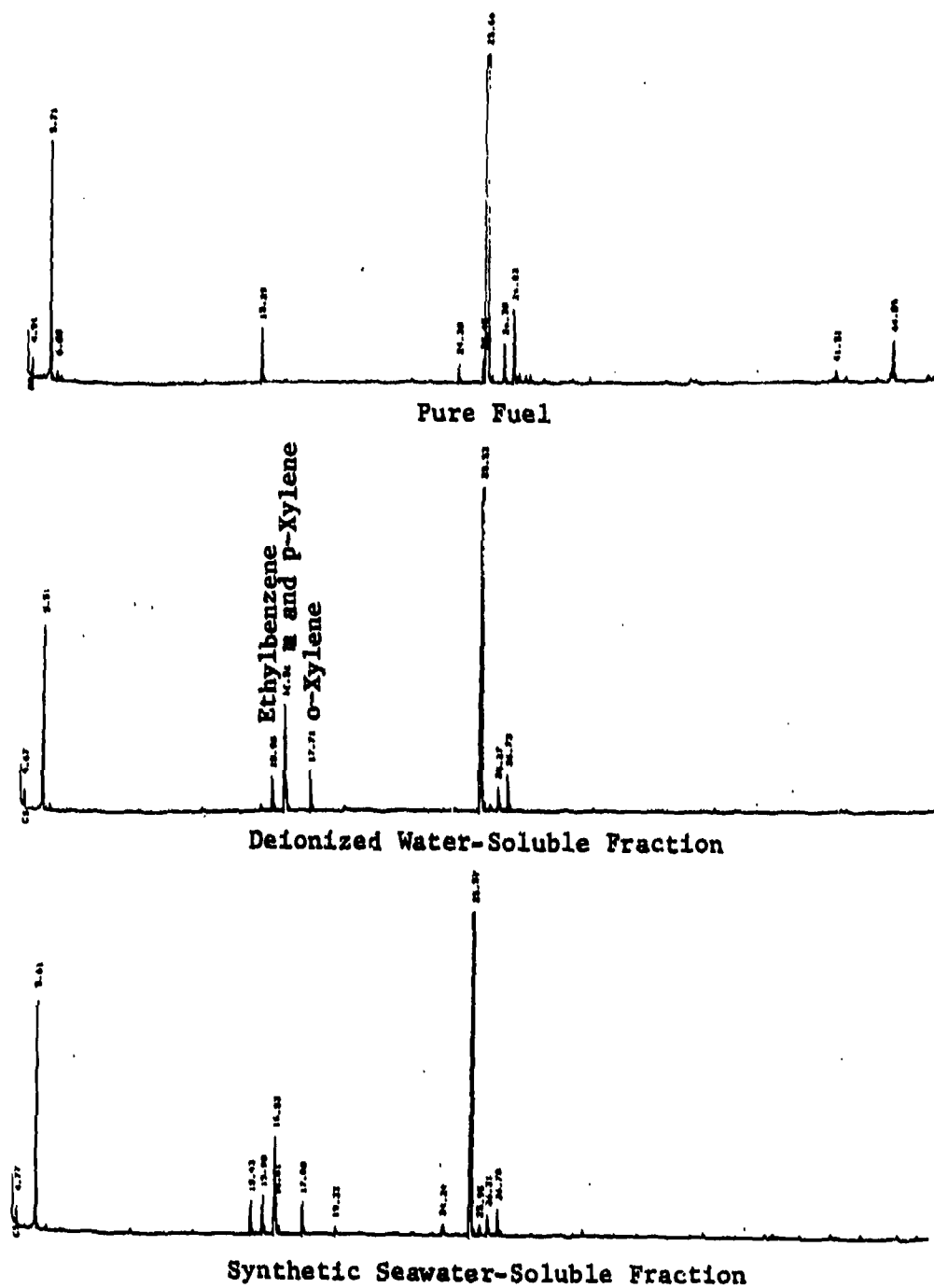
Figure C-14. GC Traces of JP-10 in CS_2

125
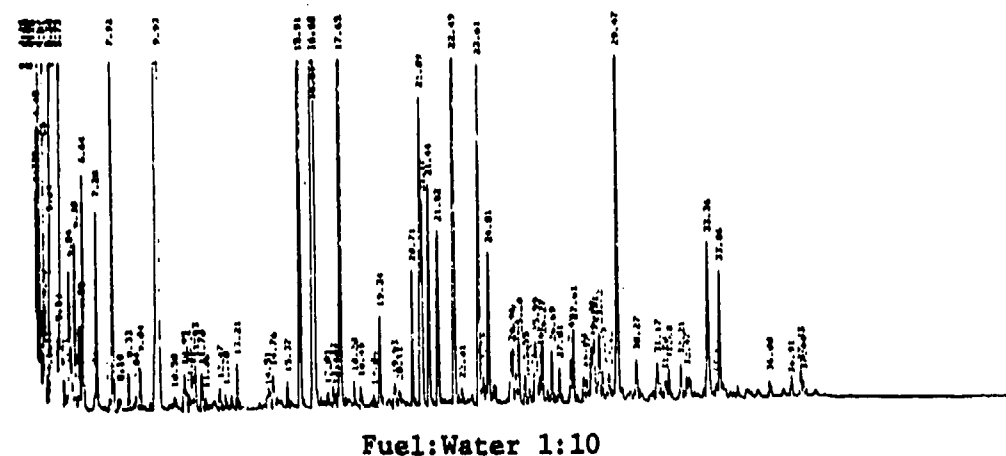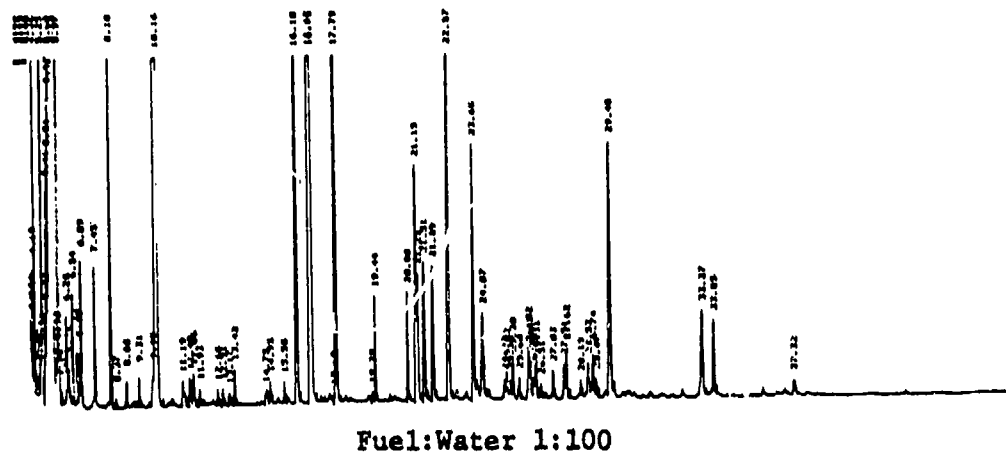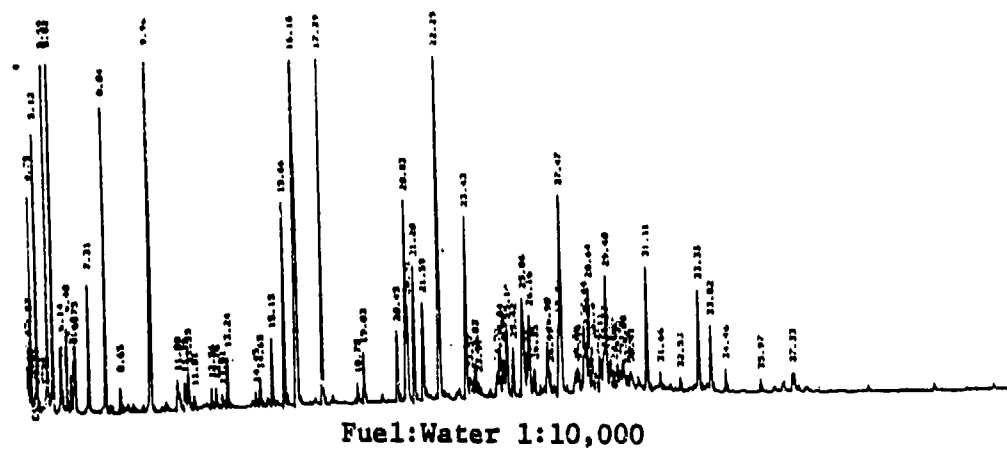
Figure C-15. Deionized Water-Soluble Fraction of JP-4
[Equilibrated at Three Fuel-to-Water Ratios $(20^{O}C)$]

Fuel:Water 1:10,000

Fuel:Water 1:100

Fuel:Water 1:10

Figure C-16. Synthetic Seawater-Soluble Fraction of JP-4
Equilibrated at Three Fuel-to-Water Ratios (20°C)

127
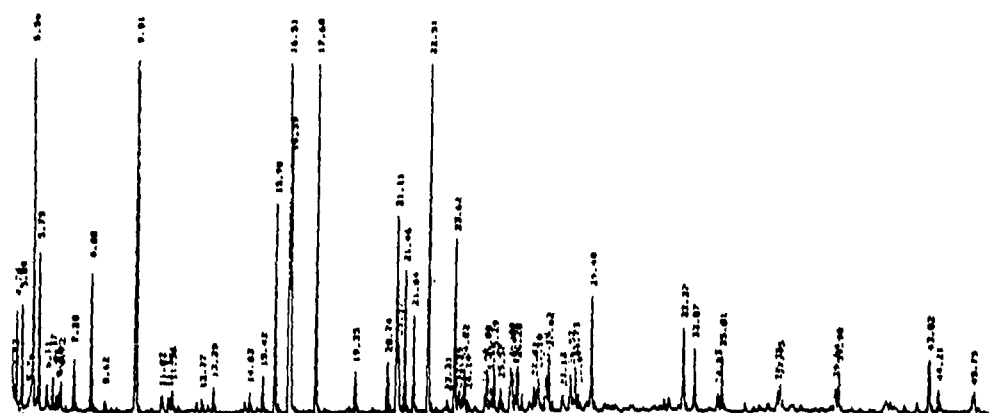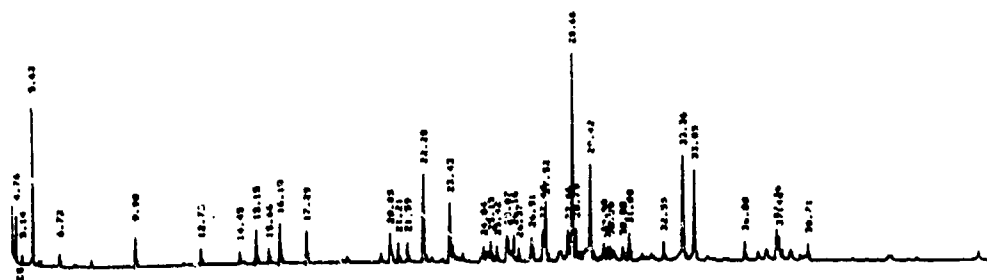
Figure C-17. Deionized Water-Soluble Fraction of JP 8
Equilibrated at Three Fuel-to-Water Ratios (20°C)

128
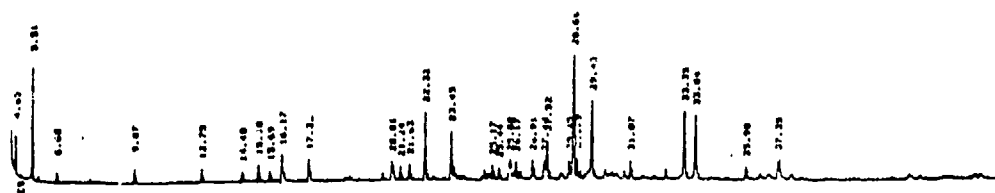
Figure C-18. Synthetic Seawater-Soluble Fraction of JP-8
Equilibrated at Three Fuel-to-Water Ratios (20°C)
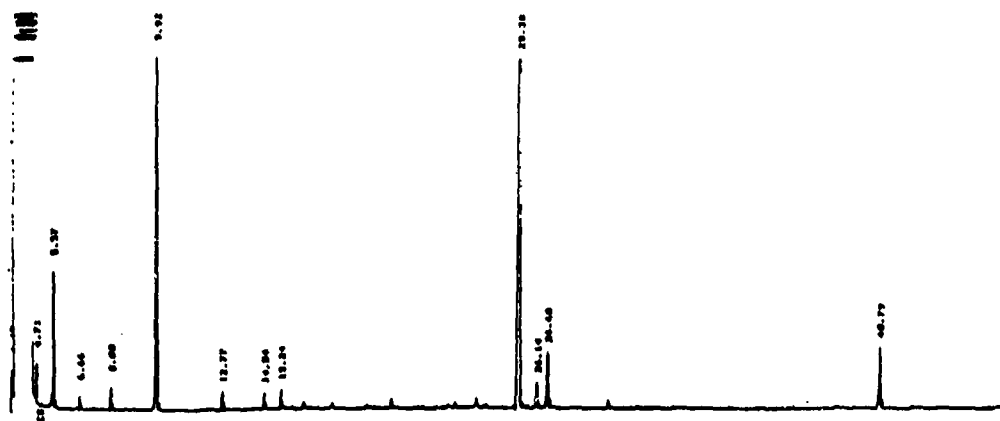
Fuel:Water 1:10,000
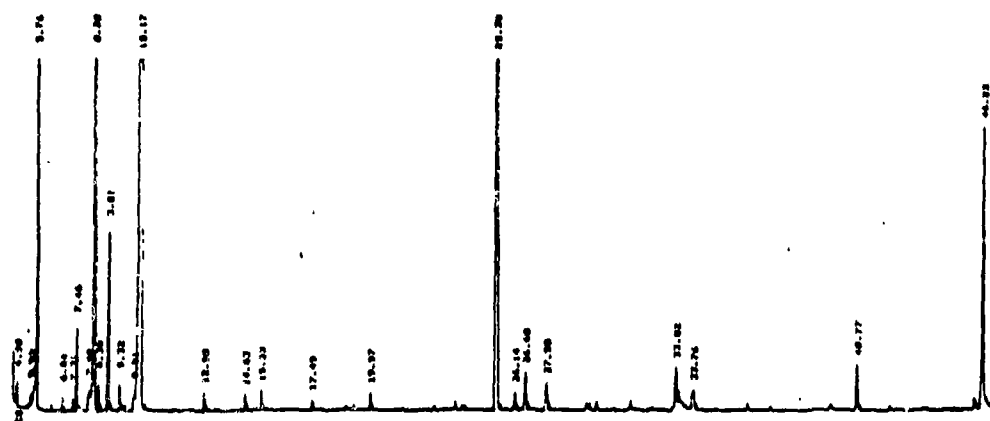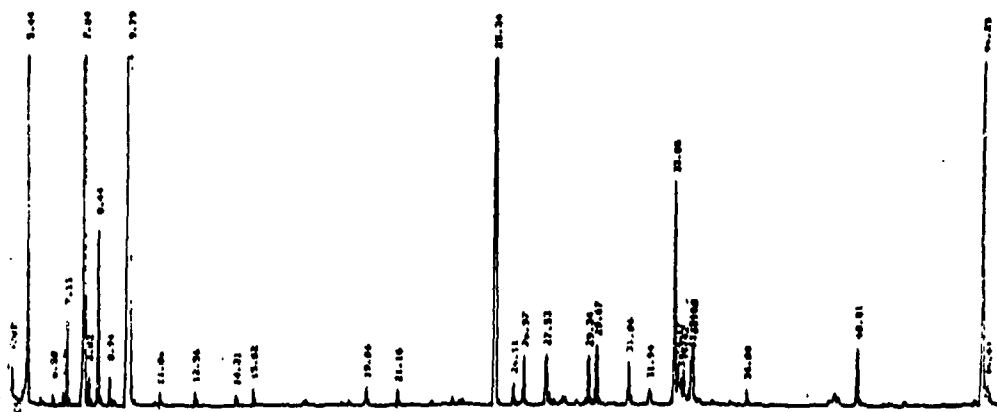
Fuel:Water 1:100

Fuel:Water 1:10

Figure C-19. Deionized Water-Soluble Fraction of JP-9
Equilibrated at Three Fuel-to-Water Ratios (20°C)

130

Figure C-20. Synthetic Seawater-Soluble Fraction of JP-9
Equilibrated at Three Fuel-to-Water Ratios (20°C)

131
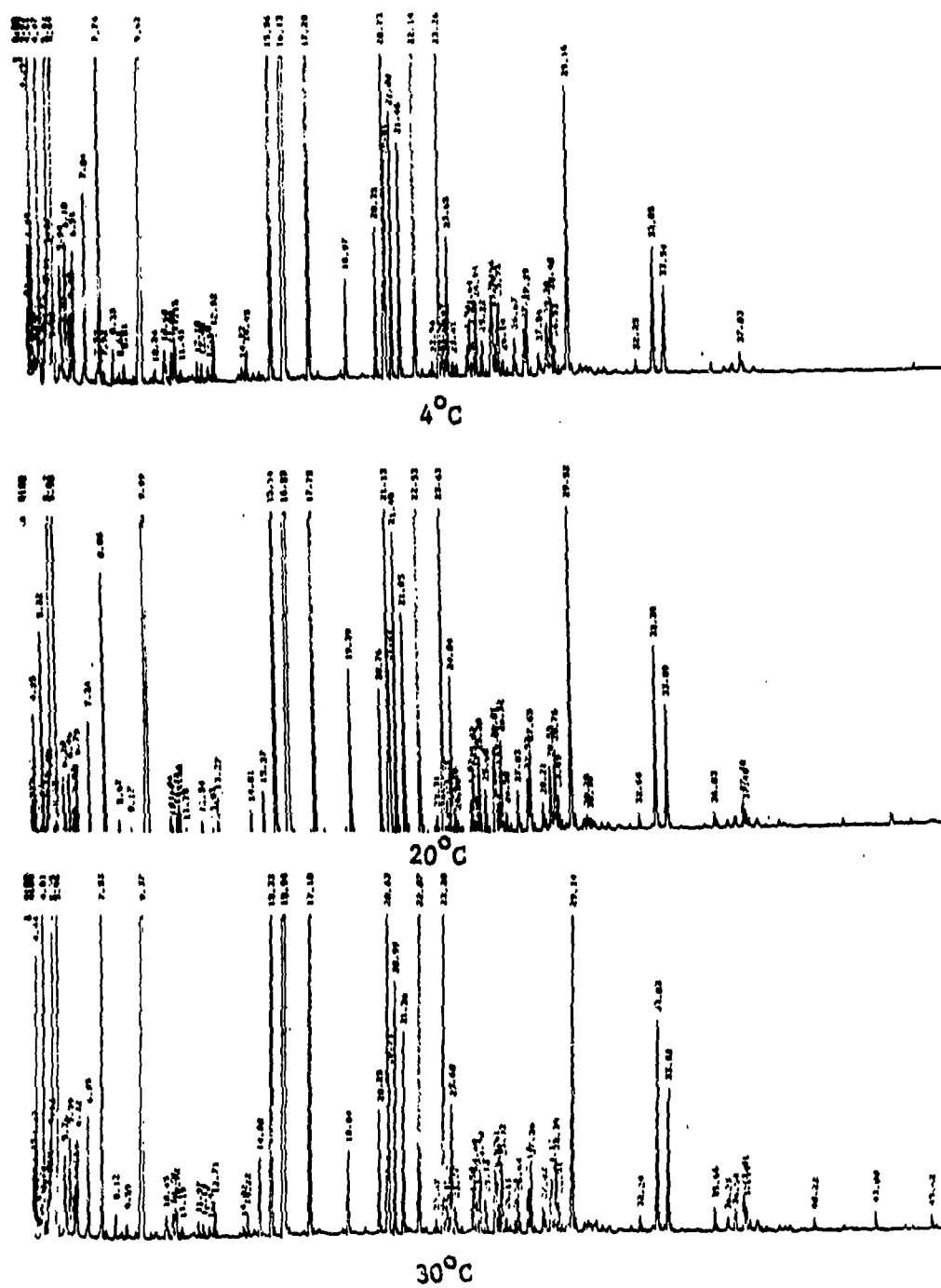
Figure C-21. Deionized Water-Soluble Fraction of JP-4
Equilibrated at three Temperatures (fuel:water 1:1000)

132
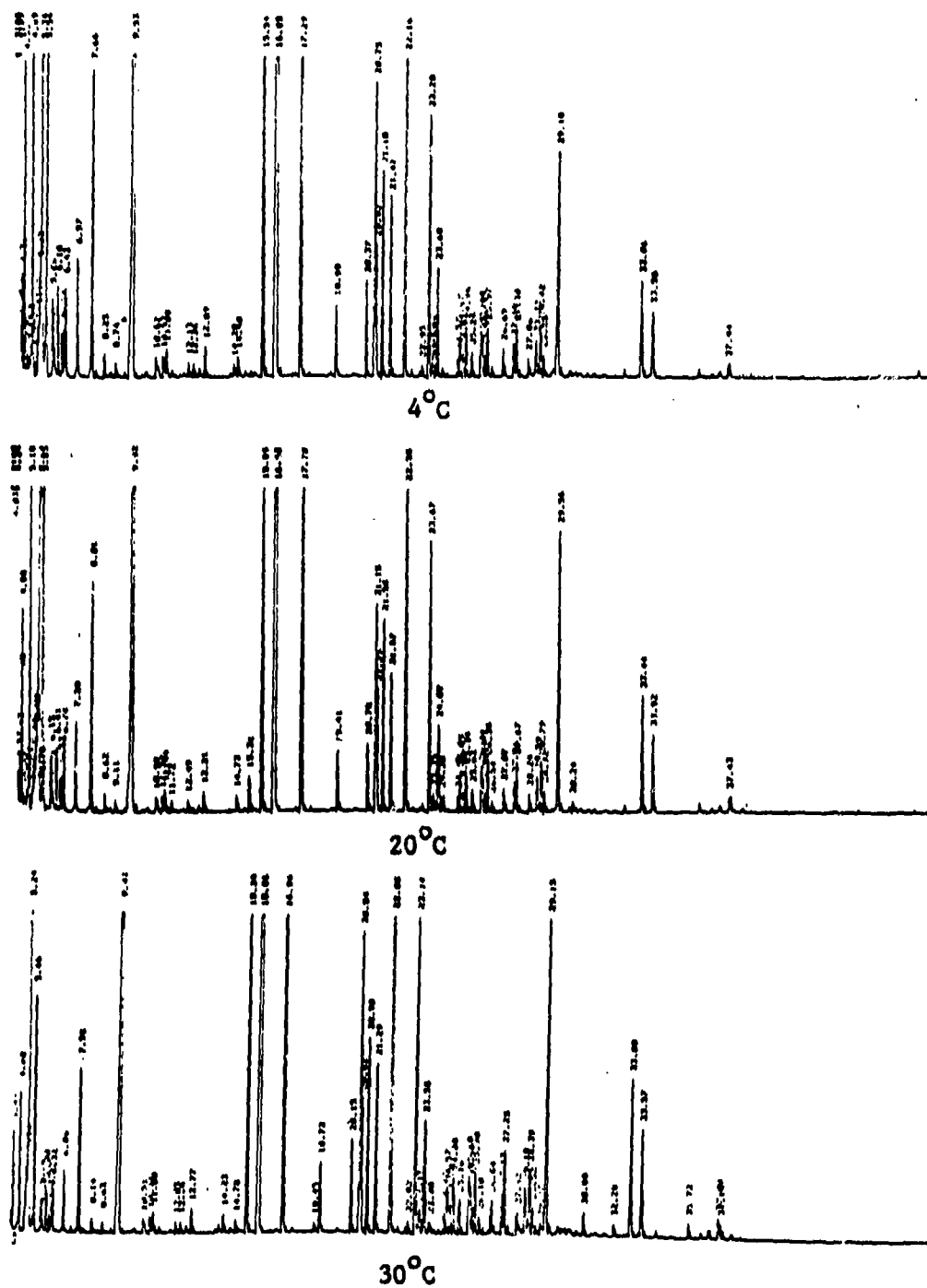
Figure C-22. Synthetic Seawater-Soluble Fraction of JP-4
Equilibrated at Three Temperatures (fuel:water 1:1000)
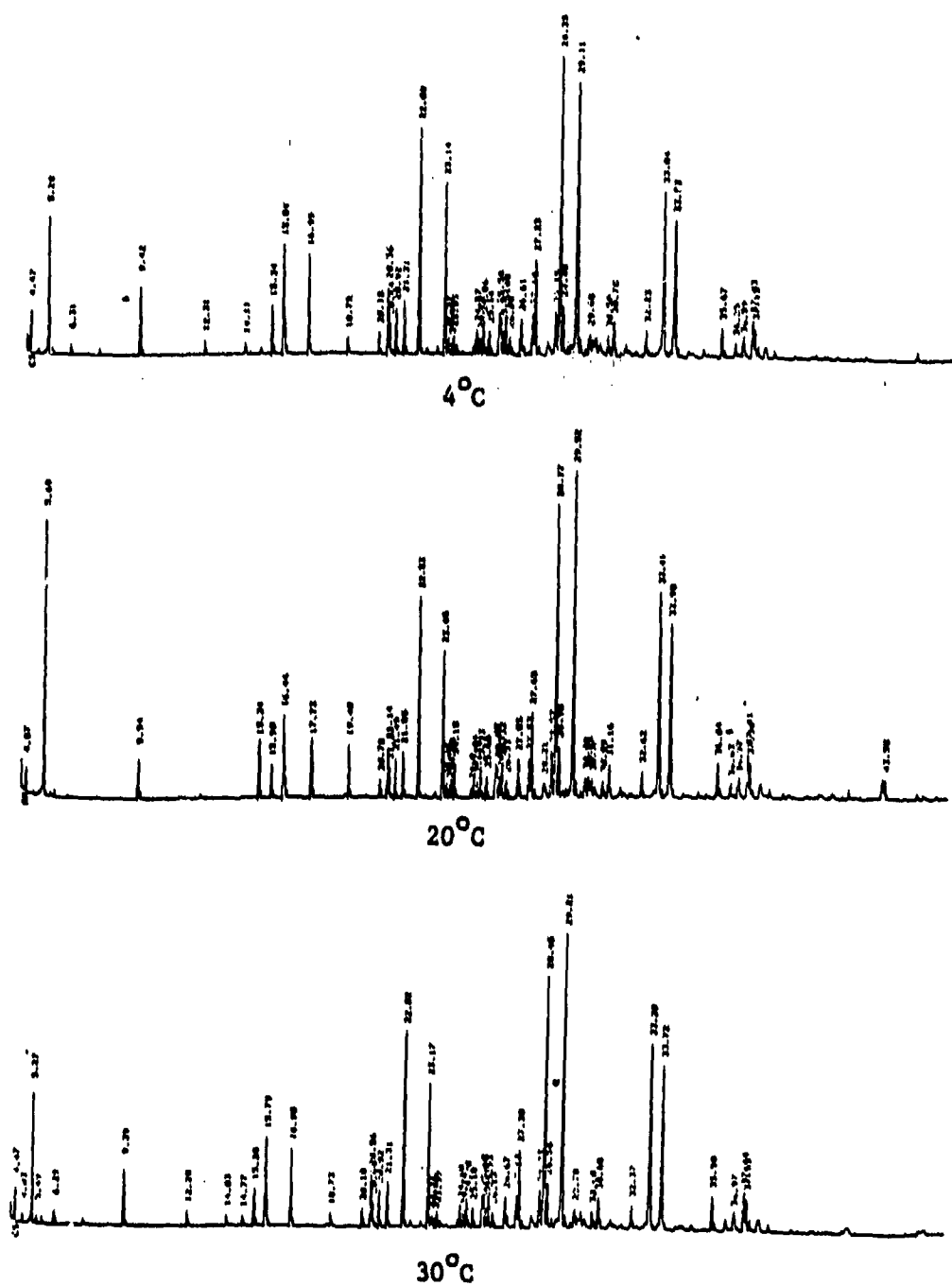
Figure C-23. Deionized Water-Soluble Fraction of JP-8
Equilibrated at Three Temperatures (fuel:water 1:1000)
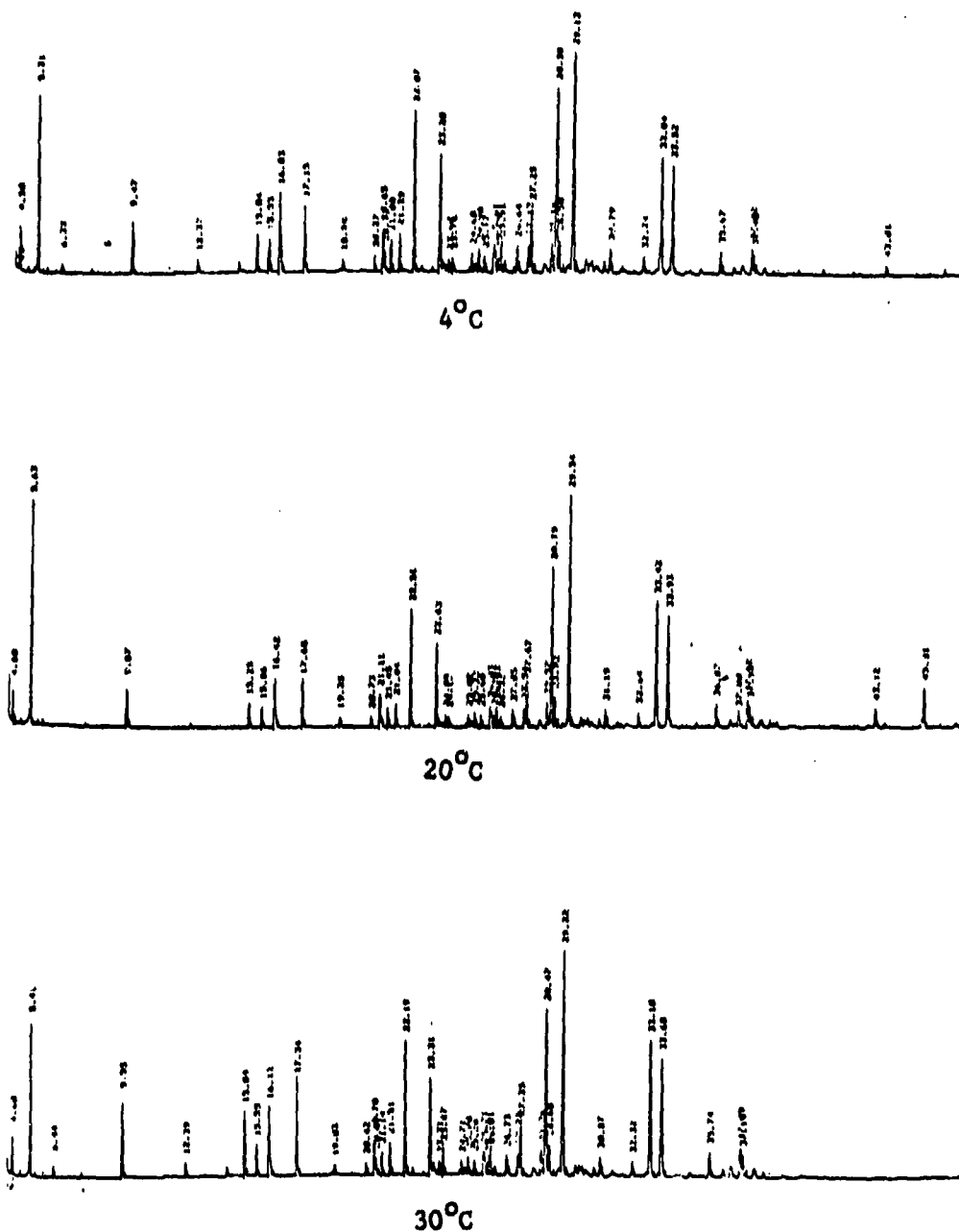
Figure C-24. Synthetic Seawater-Soluble Fraction of JP-8
Equilibrated at Three Temperatures (fuel:water 1:1000)

Figure C-25. Deionized Water-Soluble Fraction of JP-9
Equilibrated at Three Temperatures (fuel:water 1:1000)

Figure C-26. Synthetic Seawater-Soluble Fraction of JP-9
Equilibrated at Three Temperatures (fuel:water 1:1000)

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TABLE C-1. CONCENTRATIONS OF WATER-SOLUBLE COMPONENTS OF JP-4 (mg liter^{-1})

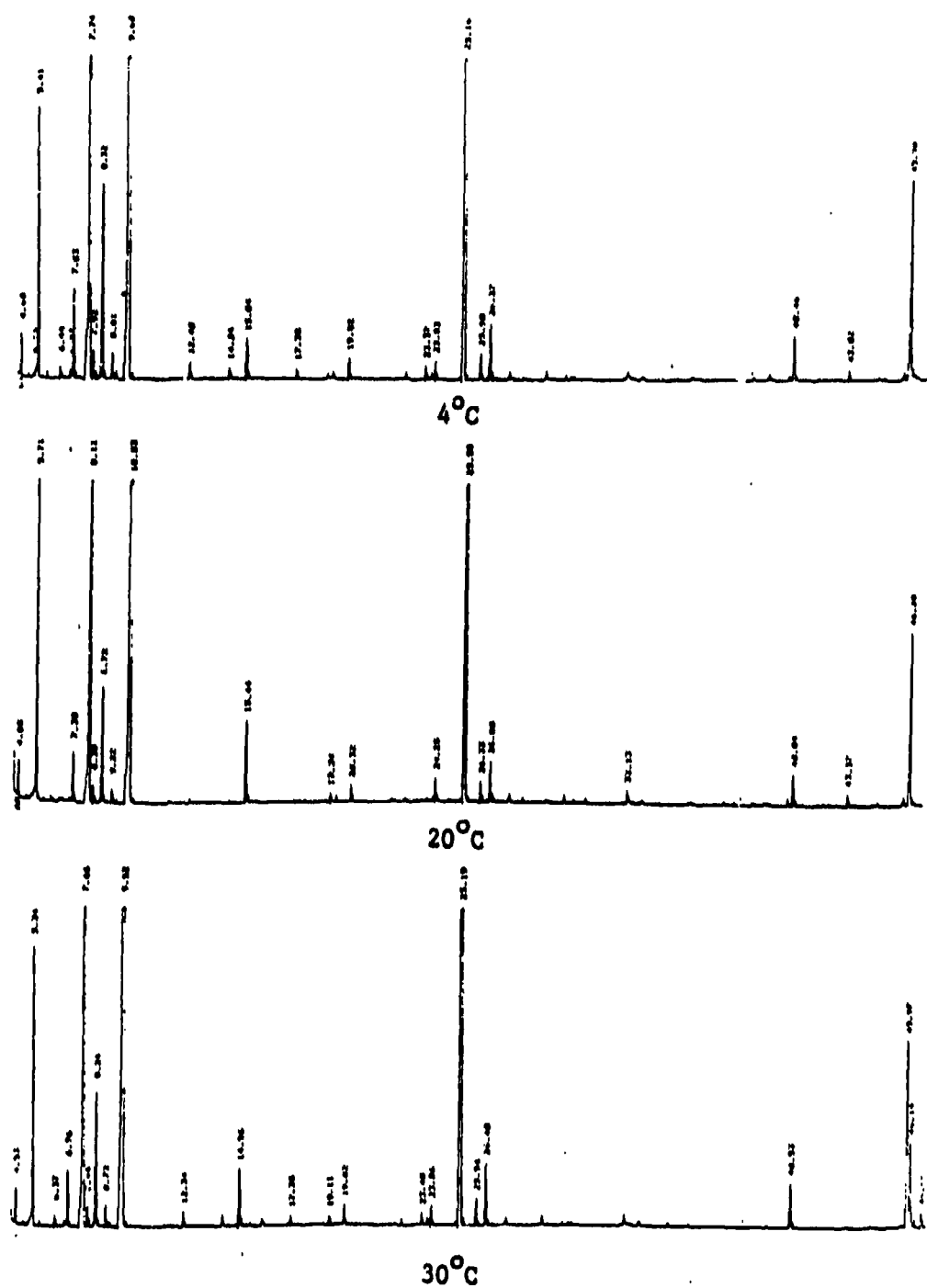|	1:10		1:100		1:1000						1:10,000	
Fuel Component	Deion.[a] (20°C)	Sea.[b] (20°C)	Deion. (20°C)	Sea. (20°C)	Deion. (4°C)	Sea. (4°C)	Deion. (20°C)	Sea. (20°C)	Deion. (30°C)	Sea. (30°C)	Deion. (20°C)	Sea. (20°C)
Methylcyclopentane	0.44	0.36	0.33	0.19	0.26	0.22	0.10	0.15	0.17	0.08	0.13	0.04
Benzene	9.82	9.06	6.99	4.86	1.41	1.50	1.55	1.32	1.33	0.94	0.07	0.02
Cyclohexane	0.65	0.54	0.48	0.32	0.46	0.39	0.19	0.25	0.31	0.14	0.22	0.07
2-Methylhexane	0.11	0.07	0.07	0.04	0.08	0.07	0.05	0.05	0.05	0.03	0.06	0.02
3-Methylhexane	0.08	0.06	0.06	0.04	0.07	0.05	0.04	0.04	0.05	0.02	0.05	0.01
trans-1,3-Dimethylcyclopentane	0.04	0.03	0.04	0.02	0.04	0.03	0.02	0.02	0.02	0.01	0.03	0.01
cis-1,3-Dimethylcyclopentane	0.05	0.04	0.04	0.03	0.04	0.03	0.02	0.02	0.03	0.03	0.03	0.01
cis-1,2-Dimethylcyclopentane	0.13	0.11	0.10	0.06	0.07	0.06	0.05	0.04	0.05	0.03	0.05	0.01
n-Heptane	0.13	0.11	0.13	0.07	0.13	0.10	0.09	0.07	0.09	0.05	0.11	0.02
Methylcyclohexane	0.33	0.26	0.30	0.18	0.31	0.26	0.24	0.19	0.23	0.12	0.24	0.08
Toluene	8.45	7.09	7.79	4.95	3.78	3.50	3.71	3.00	3.23	2.64	0.70	0.50
cis-1,3-Dimethylcyclohexane	0.04	0.03	0.02	0.01	0.04	0.03	0.04	0.01	0.02	0.02	0.05	0.01
n-Octane	0.03	0.02	0.02	0.01	0.03	0.02	0.03	0.01	0.02	0.02	0.03	0.01
Ethylbenzene	0.67	0.53	0.64	0.40	0.54	0.46	0.59	0.38	0.44	0.42	0.17	0.12
m-Xylene	2.01	1.41	1.83	1.16	{1.97}	1.30	1.89	1.06	1.28	1.22	0.55	0.35
p-Xylene	0.41	0.46	0.49	0.33	{1.97}	0.37	0.36	0.31	0.35	0.34	0.10	0.11
o-Xylene	1.21	0.95	1.17	0.74	0.91	0.79	1.08	0.67	0.78	0.78	0.27	0.21
Isopropylbenzene	0.07	0.05	0.06	0.03	0.07	0.05	0.13	0.04	0.05	0.05	0.04	0.02
n-Propylbenzene	0.08	0.06	0.07	0.04	0.08	0.07	0.10	0.05	0.07	0.07	0.05	0.04
1-Methyl-3-ethylbenzene	0.28	0.21	0.26	0.16	0.29	0.23	0.36	0.18	0.23	0.24	0.17	0.12
1-Methyl-4-ethylbenzene	0.11	0.08	0.10	0.06	0.12	0.09	0.15	0.08	0.10	0.10	0.07	0.05
1,3,5-Trimethylbenzene	0.18	0.12	0.16	0.09	0.18	0.14	0.23	0.11	0.15	0.16	0.12	0.08
1-Methyl-2-ethylbenzene	0.16	0.12	0.15	0.09	0.16	0.12	0.20	0.10	0.13	0.14	0.08	0.05
1,2,4-Trimethylbenzene	0.67	0.49	0.63	0.38	0.68	0.53	0.87	0.44	0.57	0.60	0.40	0.28
n-Decane	0.30	0.21	0.27	0.16	0.29	0.23	0.37	0.19	0.25	0.26	0.15	0.11
1,2,3-Trimethylbenzene	0.02	<0.01	<0.01	<0.01	0.02	0.01	0.03	0.01	0.02	0.02	0.02	<0.01
1-Methyl-4-isopropylbenzene	0.10	0.07	0.09	0.05	0.10	0.08	0.15	0.07	0.09	0.10	0.04	0.02
1,3-Diethylbenzene	0.04	0.04	0.01	<0.01	0.02	0.01	0.02	0.01	0.01	0.01	0.01	0.01
1-Methyl-4-propylbenzene	0.03	0.02	0.02	0.01	0.04	0.03	0.05	0.02	0.03	0.04	0.04	0.02
1,3-Dimethyl-5-ethylbenzene	0.05	0.03	0.04	0.02	0.05	0.04	0.07	0.03	0.04	0.05	0.05	0.03
1-Methyl-2-n-propylbenzene	0.02	0.01	0.01	<0.01	0.03	0.01	0.04	0.01	0.02	0.03	0.03	0.01
1,4-Dimethyl-2-ethylbenzene	0.07	0.04	0.03	0.03	0.05	0.04	0.07	0.03	0.04	0.05	0.05	0.03
1,2-Dimethyl-4-ethylbenzene	0.06	0.02	0.04	0.01	0.06	0.05	0.07	0.03	0.05	0.06	0.05	0.03
1,2-Dimethyl-3-ethylbenzene	0.02	0.01	0.02	0.01	0.03	0.02	0.04	0.01	0.02	0.03	0.02	0.01
n-Undecane	0.03	0.01	0.02	0.01	0.04	0.02	0.07	0.03	0.03	0.03	0.03	0.02
1,2,3,4-Tetramethylbenzene	0.05	0.02	0.03	0.02	0.06	0.03	0.06	0.03	0.04	0.04	0.03	0.02
Tetralin	0.02	0.01	0.01	<0.01	0.02	0.02	0.03	0.02	0.02	0.02	0.01	0.01
Naphthalene	0.39	0.29	0.31	0.22	0.27	0.22	0.41	0.24	0.30	0.32	0.10	0.08
2-Methylnaphthalene	0.16	0.11	0.11	0.05	0.12	0.09	0.19	0.10	0.17	0.15	0.10	0.06
1-Methylnaphthalene	0.08	0.06	0.06	0.05	0.08	0.06	0.13	0.06	0.11	0.10	0.06	0.04

[a] Deion. = deionized water
[b] Sea. = artificial seawater

TABLE C-2.   CONCENTRATIONS OF WATER-SOLUBLE COMPONENTS OF JP-5 (mg liter^{-1})

Fuel Component	Fuel-to-Water Ratio 1:1000	
	Deionized Water (20°C)	Artificial Seawater (20°C)
Toluene	0.06	0.03
Ethylbenzene	0.03	0.01
m-Xylene and p-xylene	0.16	0.09
o-Xylene	0.09	0.06
Isopropylbenzene	0.04	<0.01
n-Propylbenzene	0.01	0.01
1-Methyl-3-ethylbenzene	0.05	0.03
1-Methyl-4-ethylbenzene	0.02	0.01
1,3,5-Trimethylbenzene	0.05	0.03
1-Methyl-2-ethylbenzene	0.04	0.02
1,2,4-Trimethylbenzene	0.20	0.12
n-Decane	0.14	0.08
1,2,3-Trimethylbenzene	0.01	<0.01
1-Methyl-3-isopropylbenzene	0.01	<0.01
1-Methyl-4-isopropylbenzene	0.02	<0.01
1,3-Diethylbenzene	0.01	<0.01
1-Methyl-4-propylbenzene	0.02	0.01
1,3-Dimethyl-5-ethylbenzene	0.04	0.02
1-Methyl-2-n-propylbenzene	0.02	0.01
1,4-Dimethyl-2-ethylbenzene	0.03	0.01
1,2-Dimethyl-4-ethylbenzene	0.03	0.02
1,2-Dimethyl-3-ethylbenzene	0.03	0.01
n-Undecane	0.06	0.03
1,2,3,4-Tetramethylbenzene	0.08	0.04
Tetralin	0.02	0.01
Naphthalene	0.46	0.30
2-Methylnaphthalene	0.23	0.14
1-Methylnaphthalene	0.16	0.09

TABLE C-3. CONCENTRATIONS OF WATER-SOLUBLE COMPONENTS OF JP-8 (mg liter^{-1})

| | Fuel-To-Water Ratio | | | | | | | | | | | |
| | 1:10 | | 1:100 | | 1:1000 | | | | | | 1:10,000 | |
Fuel Component	Deion.ᵃ (20°C)	Sea.ᵇ (20°C)	Deion. (20°C)	Sea. (20°C)	Deion. (4°C)	Sea. (4°C)	Deion. (20°C)	Sea. (20°C)	Deion. (30°C)	Sea. (30°C)	Deion. (20°C)	Sea. (20°C)
Toluene	0.15	0.14	0.13	0.08	0.05	0.04	0.03	0.03	0.05	0.06	0.02	0.01
Ethylbenzene	0.05	0.04	0.04	0.03	0.03	0.02	0.02	0.01	0.03	0.02	0.01	<0.01
m-Xylene and p-xylene	0.15	0.12	0.13	0.39	0.09	0.07	0.07	0.04	0.08	0.06	0.03	0.02
o-Xylene	0.11	0.09	0.10	0.07	0.06	0.05	0.05	0.03	0.06	0.05	0.01	0.01
Isopropylbenzene	0.01	<0.01	0.01	<0.01	0.01	<0.01	0.04	<0.01	<0.01	<0.01	<0.01	<0.01
n-Propylbenzene	0.01	0.01	0.01	0.01	0.01	0.01	0.01	<0.01	0.01	0.01	<0.01	<0.01
1-Methyl-3-ethylbenzene	0.05	0.04	0.04	{0.04}	0.04	0.03	0.03	0.02	0.03	0.02	{0.02}	{0.01}
1-Methyl-4-ethylbenzene	0.02	0.02	0.02		0.02	0.01	0.02	<0.01	0.02	0.01		
1,3,5-Trimethylbenzene	0.03	0.02	0.03	0.02	0.03	0.02	0.02	0.01	0.02	0.01	0.01	0.01
1-Methyl-2-ethylbenzene	0.04	0.03	0.04	0.02	0.03	0.02	0.03	0.01	0.03	0.02	0.01	0.01
1,2,4-Trimethylbenzene	0.20	0.16	0.18	0.11	0.16	0.11	0.15	0.08	0.15	0.10	0.07	0.06
n-Decane	0.15	0.12	0.13	0.08	0.12	0.09	0.12	0.06	0.11	0.08	0.05	0.04
1-Methyl-4-isopropylbenzene	0.01	0.01	<0.01	0.01	0.01	<0.01	0.01	<0.01	0.01	0.01	<0.01	<0.01
1,3-Diethylbenzene	0.01	0.01	0.01	<0.01	<0.01	<0.01	0.02	0.01	<0.01	<0.01	<0.01	<0.01
1-Methyl-2-n-propylbenzene	0.01	0.01	0.01	0.01	0.01	0.01	0.01	<0.01	0.01	0.01	0.01	<0.01
1,4-Dimethyl-2-ethylbenzene	0.03	0.04	0.02	0.03	0.05	0.03	0.02	0.02	0.02	0.02	0.02	<0.01
1,2-Dimethyl-4-ethylbenzene	0.03	0.02	0.03	0.01	0.03	0.02	0.03	0.01	0.02	0.01	0.01	0.01
1,2-Dimethyl-3-ethylbenzene	0.03	0.02	0.02	0.01	0.03	0.02	0.02	0.01	0.02	0.01	0.01	0.01
n-Undecane	0.03	0.02	0.02	0.01	0.03	0.02	0.07	0.01	0.02	0.01	0.02	<0.01
1,2,3,4-Tetramethylbenzene	0.29	0.21	0.24	0.13	0.25	0.17	0.25	0.12	0.23	0.15	0.15	0.12
Tetralin	0.05	0.04	0.04	0.02	0.04	0.03	0.04	0.02	0.04	0.03	0.02	0.02
Naphthalene	0.41	0.34	0.31	0.22	0.25	0.19	0.31	0.20	0.28	0.22	0.06	0.06
n-Dodecane	0.09	0.08	0.03	<0.01	<0.01	<0.01	0.02	0.01	0.02	0.01	0.02	0.01
2-Methylnaphthalene	0.34	0.27	0.17	0.10	0.15	0.11	0.19	0.11	0.18	0.13	0.08	0.06
1-Methylnaphthalene	0.15	0.12	0.12	0.08	0.13	0.09	0.16	0.10	0.15	0.11	0.07	0.05

ᵃDeion. = deionized water.
ᵇSea. = artificial seawater.

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TABLE C-4. DATA FOR THE ERROR ANALYSIS OF THE WATER-SOLUBLE FRACTION OF JP-4 (mg liter^{-1})

	Sample 1				Sample 2			
	Extraction 1		Extraction 2		Extraction 1		Extraction 2	
Fuel Component	Analysis 1	Analysis 2	Analysis 1	Analysis 2	Analysis 1	Analysis 2	Analysis 1	Analysis 2
Methylcyclopentane	0.10	0.10	0.09	0.08	0.06	0.06	0.06	0.07
Benzene	0.87	0.87	0.85	0.71	0.78	0.78	0.65	0.72
Cyclohexane	0.19	0.18	0.18	0.15	0.12	0.13	0.11	0.12
2-Methylhexane	0.04	0.04	0.05	0.03	0.03	0.03	0.02	0.03
3-Methylhexane	0.03	0.03	0.03	0.03	0.03	0.03	0.02	0.02
trans-1,3-Dimethylcyclopentane	0.02	0.02	0.02	0.01	0.01	0.01	0.01	0.01
cis-1,3-Dimethylcyclopentane	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02
cis-1,2-Dimethylcyclopentane	0.04	0.04	0.03	0.03	0.03	0.03	0.03	0.03
n-Heptane	0.07	0.07	0.04	0.05	0.05	0.04	0.04	0.05
Methylcyclohexane	0.18	0.16	0.14	0.13	0.14	0.13	0.12	0.13
Toluene	2.62	2.57	2.36	2.13	2.48	2.38	2.13	2.29
cis-1,3-Dimethylcyclohexane	0.03	0.03	0.03	0.02	0.03	0.03	0.02	0.03
n-Octane	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02
Ethylbenzene	0.41	0.40	0.36	0.33	0.41	0.40	0.36	0.39
m-Xylene and p-xylene	1.50	1.48	1.34	1.22	1.56	1.50	1.34	1.47
o-Xylene	0.71	0.70	0.64	0.58	0.74	0.72	0.64	0.70
Isopropylbenzene	0.05	0.05	0.04	0.04	0.06	0.05	0.05	0.05
n-Propylbenzene	0.07	0.07	0.06	0.05	0.07	0.07	0.06	0.07
1-Methyl-3-ethylbenzene	0.23	0.23	0.20	0.19	0.25	0.24	0.22	0.24
1-Methyl-4-ethylbenzene	0.10	0.09	0.09	0.08	0.11	0.10	0.09	0.10
1,3,5-Trimethylbenzene	0.15	0.14	0.13	0.12	0.16	0.15	0.14	0.15
1-Methyl-2-Ethylbenzene	0.13	0.13	0.11	0.10	0.14	0.13	0.12	0.13
1,2,4-Trimethylbenzene	0.56	0.55	0.50	0.45	0.61	0.59	0.53	0.58
sec-Butylbenzene	<0.01	0.01	<0.01	<0.01	0.01	0.01	<0.01	<0.01
n-Decane	0.24	0.23	0.21	0.19	0.26	0.25	0.27	0.25
1,2,3-Trimethylbenzene	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02
1-Methyl-3-isopropylbenzene	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
1-Methyl-4-isopropylbenzene	0.09	0.08	0.07	0.07	0.09	0.09	0.08	0.09
1,3-Diethylbenzene	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
1-Methyl-4-propylbenzene	0.03	0.03	0.03	0.02	0.03	0.03	0.03	0.03
1,3-Dimethyl-5-ethylbenzene	0.04	0.04	0.04	0.04	0.05	0.04	0.04	0.05
1-Methyl-2-n-propylbenzene	0.02	0.02	0.02	0.02	0.03	0.02	0.02	0.02
1,4-Dimethyl-2-ethylbenzene	0.07	0.07	0.06	0.05	0.05	0.05	0.04	0.05
1,2-Dimethyl-4-ethylbenzene	0.04	0.04	0.05	0.04	0.05	0.05	0.05	0.05
1,2-Dimethyl-3-ethylbenzene	0.02	0.02	0.01	0.02	0.02	0.02	0.02	0.02
n-Undecane	0.05	0.03	0.04	0.02	0.03	0.03	0.03	0.02
1,2,3,4-Tetramethylbenzene	0.04	0.04	0.03	0.03	0.04	0.04	0.04	0.04
Tetraline	0.02	0.02	0.02	0.01	0.02	0.02	0.02	0.02
Naphthalene	0.26	0.25	0.22	0.21	0.27	0.27	0.25	0.32
2-Methylnaphthalene	0.12	0.12	0.11	0.16	0.13	0.13	0.12	0.27
1-Methylnaphthalene	0.08	0.08	0.07	0.07	0.09	0.07	0.08	0.13

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Figure C-27. Volatilization of JP-4 Fuel Components From Deionized Water

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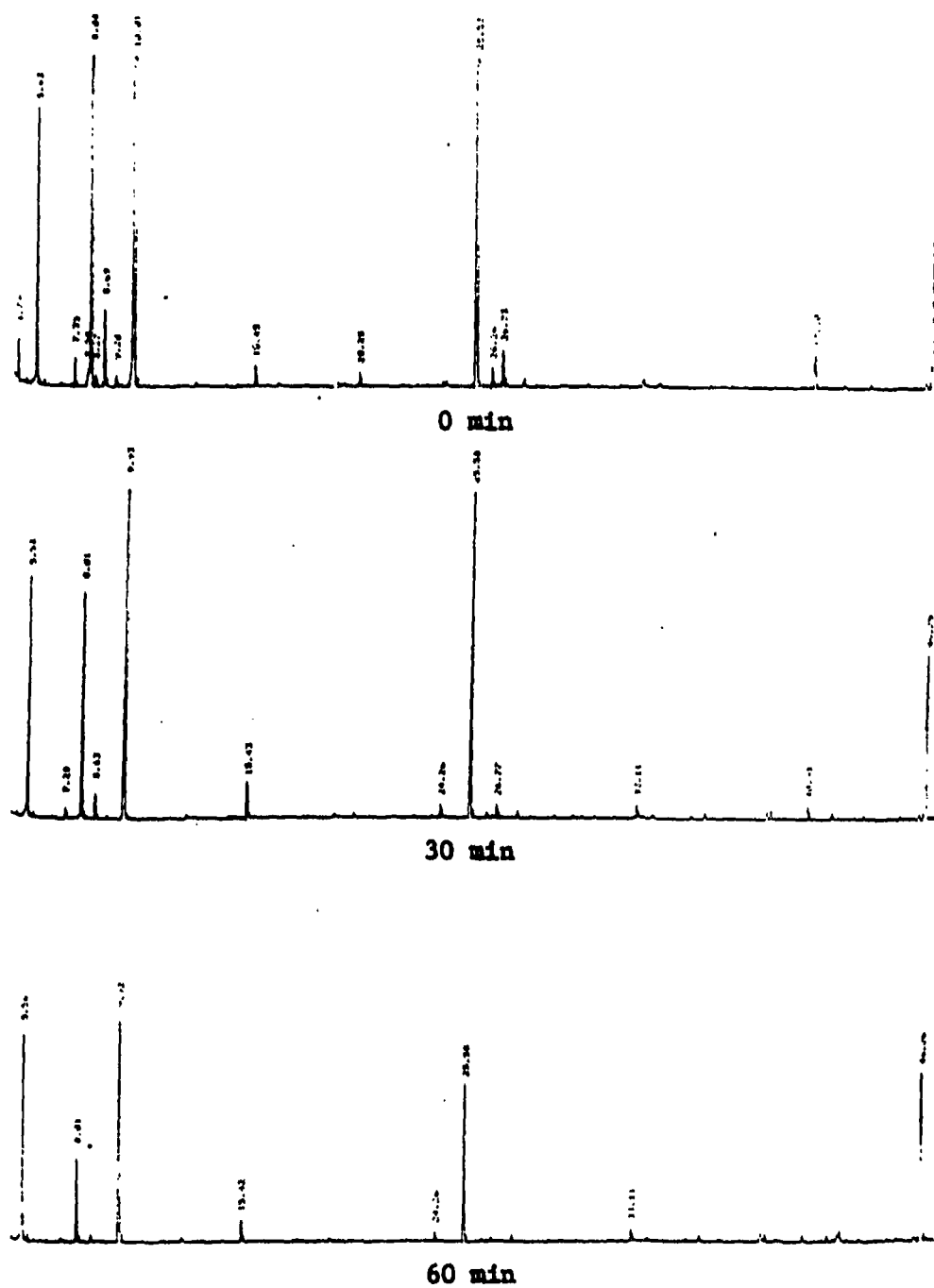Figure C-28. Volatilization of JP-8 Fuel Components From Deionized Water

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Figure C-29. Volatilization of JP-9 Fuel Components From Deionized Water

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TABLE C-5. VOLATILIZATION RATE DATA FOR JP-4

Fuel Component	k_v^C/k_v^O			Average k_v^C/k_v^O
	$k_v^O = 2.81 \ hr^{-1}$	$k_v^O = 5.82 \ hr^{-1}$	$k_v^O = 15.1 \ hr^{-1}$	
Benzene	0.52	0.32	0.30	0.38 ± 0.12
Cyclohexane	0.65	0.50	0.55	0.57 ± 0.08
Toluene	0.64	0.50	0.80	0.65 ± 0.15
Ethylbenzene	0.64	0.51	0.56	0.57 ± 0.07
m-Xylene and p-xylene	0.61	0.48	0.86	0.65 ± 0.19
o-Xylene	0.58	0.46	0.73	0.59 ± 0.14
Isopropylbenzene	0.68	0.57	0.66	0.64 ± 0.06
n-Propylbenzene	0.78	0.59	0.59	0.65 ± 0.11
1-Methyl-3-ethylbenzene	0.60	0.49	0.54	0.54 ± 0.06
1-Methyl-4-ethylbenzene	0.65	0.50	0.54	0.56 ± 0.08
1,3,5-Trimethylbenzene	0.62	0.49	0.52	0.54 ± 0.07
1-Methyl-2-ethylbenzene	0.62	0.50	0.52	0.55 ± 0.06
1,2,4-Trimethylbenzene	0.57	0.45	0.74	0.59 ± 0.15
n-Decane	0.56	0.43	0.46	0.48 ± 0.07
1,3-Dimethyl-5-ethylbenzene	0.73	0.59	0.55	0.62 ± 0.09
1,2-Dimethyl-4-ethylbenzene	0.74	0.65	0.65	0.68 ± 0.05
n-Undecane	0.72	0.46	0.56	0.58 ± 0.13
1,2,3,4-Tetramethylbenzene	0.54	0.42	0.46	0.47 ± 0.06
Naphthalene	0.30	0.24	0.51	0.35 ± 0.14
2-Methylnaphthalene	0.32	0.26	0.58	0.39 ± 0.17
1-Methylnaphthalene	0.27	0.21	0.25	0.24 ± 0.03

TABLE C-6. VOLATILIZATION RATE DATA FOR JP-8

Fuel Component	k_v^C/k_v^O			Average k_v^C/k_v^O
	$k_v^O = 2.71 \ hr^{-1}$	$k_v^O = 4.33 \ hr^{-1}$	$k_v^O = 17.0 \ hr^{-1}$	
Toluene	0.37	0.74		0.56 ± 0.26
m-Xylene and p-xylene	0.28	0.76	0.82	0.62 ± 0.30
o-Xylene	0.29	0.75	0.51	0.52 ± 0.23
1-Methyl-3-ethylbenzene	0.35	0.68		0.52 ± 0.23
1-Methyl-2-ethylbenzene	0.30	0.66		0.48 ± 0.25
1,2,4-Trimethylbenzene	0.26	0.62	0.48	0.45 ± 0.18
n-Decane	0.26	0.59	0.48	0.44 ± 0.17
n-Undecane	0.24	0.66	0.60	0.50 ± 0.23
1,2,3,4-Tetramethylbenzene	0.24	0.47	0.44	0.38 ± 0.13
Tetralin	0.24	0.48	0.38	0.37 ± 0.12
Naphthalene	0.22	0.28	0.20	0.23 ± 0.04
2-Methylnaphthalene	0.22	0.32	0.25	0.26 ± 0.05
1-Methylnaphthalene	0.21	0.25	0.20	0.22 ± 0.03

7 days

14 days

21 days

Figure C-30. Photolysis of JP-4 Fuel Components in Deionized Water

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7 days

14 days

21 days

Figure C-31. Photolysis of JP-4 Fuel Components in Pond Water

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Figure C-32. Photolysis of JP-4 Fuel Components in Seawater

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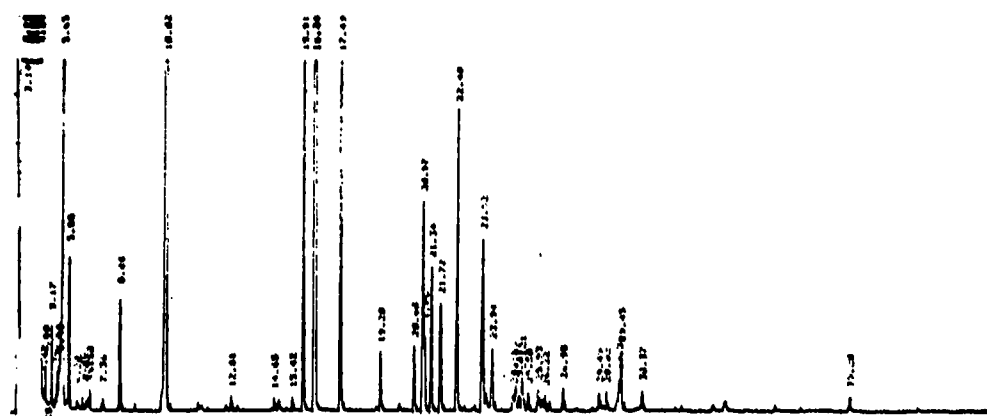
TABLE C-7. PHOTOLYSIS OF THE WATER-SOLUBLE COMPONENTS OF JP-4

Fuel Component Concentration (mg liter^{-1})

Fuel Component	Deionized Water				Artificial Seawater				Pond Water			
	Dark Control*	7 Days	14 days	21 Days	Dark Control	7 Days	14 Days	21 Days	Dark Control	7 Days	14 Days	21 Days
Methylcyclopentane	0.11	0.09	0.09	0.14	0.04	0.06	0.04	0.04	0.15	0.18	0.23	0.18
Benzene	1.15	0.68	0.82	0.98	0.76	0.88	0.67	0.65	1.24	1.16	1.20	1.32
Cyclohexane	0.23	0.15	0.17	0.26	0.10	0.11	0.09	0.08	0.31	0.28	0.34	0.34
2-Methylhexane	0.01	0.01	0.01	0.02	<0.01	0.02	0.01	—	0.02	0.03	0.03	0.03
3-Methylhexane	0.01	0.01	0.01	0.02	<0.01	0.01	0.01	0.01	0.02	0.03	0.04	0.03
trans-1,3-Dimethylcyclopentane	0.02	0.01	0.02	0.02	0.01	0.02	0.01	0.01	0.02	0.02	0.02	0.02
cis-1,3-Dimethylcyclopentane	0.03	0.02	0.02	0.02	0.02	0.01	0.01	0.01	0.02	0.03	0.03	0.03
cis-1,2-Dimethylcyclopentane	0.01	0.01	<0.01	0.01	0.02	0.01	0.02	0.01	0.05	0.04	0.04	0.05
n-Heptane	0.01	0.01	<0.01	0.01	<0.01	<0.01	<0.01	—	<0.01	0.03	0.02	0.01
Methylcyclohexane	0.15	0.10	0.10	0.16	0.08	0.09	0.09	0.07	0.16	0.22	0.22	0.22
Toluene	2.82	1.75	1.95	2.01	2.22	2.61	2.07	1.95	2.86	2.74	2.80	2.85
n-Octane	<0.01	<0.01	—	—	<0.01	<0.01	—	—	<0.01	<0.01	—	—
Ethylbenzene	0.40	0.25	0.27	0.25	0.36	0.42	0.33	0.30	0.40	0.40	0.41	0.40
m-Xylene and p-xylene	1.43	0.87	0.85	0.63	1.30	1.54	1.15	0.99	1.46	1.38	1.34	1.20
o-Xylene	0.74	0.45	0.48	0.37	0.70	0.79	0.63	0.58	0.75	0.68	0.68	0.65
Isopropylbenzene	0.05	0.03	0.03	0.03	0.05	0.05	0.04	0.04	0.05	0.05	0.05	0.05
n-Propylbenzene	0.06	0.04	0.04	0.04	0.05	0.07	0.05	0.05	0.06	0.06	0.06	0.06
1-Methyl-3-ethylbenzene	0.21	0.12	{0.16}	{0.08}	0.20	0.24	0.18	0.15	0.21	0.20	0.21	0.18
1-Methyl-4-ethylbenzene	0.08	0.04	0.06	0.03	0.07	0.08	0.04	0.03	0.07	0.07	0.06	0.04
1,3,5-Trimethylbenzene	0.13	0.07	0.07	0.05	0.13	0.14	0.09	0.06	0.14	0.12	0.11	0.09
1-Methyl-2-ethylbenzene	0.12	0.07	0.07	0.05	0.12	0.13	0.10	0.09	0.22	0.11	0.11	0.11
1,2,4-Trimethylbenzene	0.51	0.23	0.11	0.03	0.49	0.31	0.05	—	0.52	0.37	0.27	0.10
n-Decane	0.23	0.13	0.09	0.03	0.23	0.23	0.15	0.10	0.24	0.19	0.18	0.14
1-Methyl-4-isopropylbenzene	0.08	<0.01	<0.01	—	0.08	0.07	0.03	0.02	0.08	0.05	0.04	0.02
1,3-Diethylbenzene	0.02	0.01	—	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.02	0.04
1-Methyl-4-propylbenzene	0.02	0.01	0.01	0.01	0.02	0.01	0.02	0.02	0.02	0.02	0.02	0.02
1,3-Dimethyl-5-ethylbenzene	0.04	0.01	—	—	0.04	0.03	0.02	—	0.03	0.03	0.03	—
1-Methyl-2-n-propylbenzene	0.01	0.01	—	—	0.01	0.01	0.02	0.01	0.01	0.01	0.02	—
1,4-Dimethyl-2-ethylbenzene	0.04	0.02	—	—	0.04	0.01	—	—	0.04	0.03	0.03	—
1,2-Dimethyl-4-ethylbenzene	0.04	0.01	—	—	0.03	0.01	0.01	—	0.04	0.02	0.01	—
1,2-Dimethyl-3-ethylbenzene	0.02	0.01	—	—	0.01	0.01	—	—	0.02	0.01	0.01	—
n-Undecane	0.02	0.01	—	—	0.02	<0.01	0.01	<0.01	0.03	<0.01	—	—
1,2,3,4-Tetramethylbenzene	0.04	0.01	—	—	0.03	0.01	—	—	0.04	0.01	0.01	—
Tetralin	0.02	<0.01	—	—	0.02	<0.01	—	—	0.02	0.01	0.01	0.01
Naphthalene	0.25	0.14	0.18	0.15	0.26	0.06	<0.01	—	0.29	0.16	0.09	0.01
2-Methylnaphthalene	0.10	0.04	0.05	0.02	0.10	<0.01	<0.01	—	0.11	0.03	0.02	—
1-Methylnaphthalene	0.07	0.03	0.04	0.01	0.37	<0.01	<0.01	—	0.08	0.03	0.02	—

* Average of 7, 14 and 21 day dark control samples.

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